



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:53 AM BST

PDB ID : 6QPH
Title : Dunaliella minimal PSI complex
Authors : Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on : 2019-02-14
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

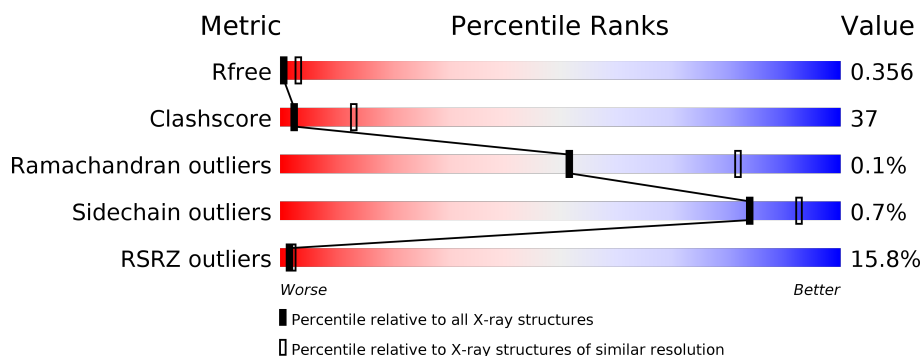
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	195	<div> <div>18%</div> <div>56%</div> <div>44%</div> </div>
2	2	211	<div> <div>16%</div> <div>61%</div> <div>39%</div> </div>
3	3	210	<div> <div>22%</div> <div>51%</div> <div>49%</div> </div>
4	4	211	<div> <div>12%</div> <div>58%</div> <div>41%</div> <div>.</div> </div>
5	A	739	<div> <div>14%</div> <div>48%</div> <div>52%</div> <div>.</div> </div>
6	B	734	<div> <div>16%</div> <div>54%</div> <div>46%</div> </div>

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Mol	Chain	Length	Quality of chain
7	C	80	
8	D	142	
9	E	64	
10	F	163	
11	J	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	LUT	1	501	-	-	-	X
12	LUT	2	501	-	-	-	X
12	LUT	3	501	-	-	-	X
12	LUT	4	501	-	-	-	X
13	XAT	2	502	X	-	-	-
13	XAT	3	502	X	-	X	X
13	XAT	4	502	X	-	-	-
14	BCR	1	503	-	-	-	X
14	BCR	1	505	-	-	-	X
14	BCR	2	503	-	-	-	X
14	BCR	3	503	-	-	X	X
14	BCR	3	504	-	-	-	X
14	BCR	4	503	-	-	-	X
14	BCR	4	505	-	-	-	X
14	BCR	A	4002	-	-	-	X
14	BCR	A	4003	-	-	-	X
14	BCR	A	4004	-	-	-	X
14	BCR	A	4005	-	-	-	X
14	BCR	A	4007	-	-	-	X
14	BCR	B	4001	-	-	-	X
14	BCR	B	4002	-	-	-	X
14	BCR	B	4003	-	-	-	X
14	BCR	B	4005	-	-	-	X
14	BCR	B	4006	-	-	-	X
14	BCR	J	4001	-	-	-	X
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	-	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	X	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	X
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	2	615	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	X	-
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	615	X	-	-	-
15	CLA	A	1012	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1013	X	-	X	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	X	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	X
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	X
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	X
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1021	X	-	X	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	X
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	X
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	X
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	X
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
21	DGD	4	811	-	-	-	X
21	DGD	J	5001	-	-	-	X
24	CL0	A	1011	X	-	X	-
25	PQN	A	2001	-	-	-	X
25	PQN	B	2002	-	-	-	X
26	SF4	C	3003	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 30870 atoms, of which 32 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	195	Total	C	N	O	S	0	0	0
			1490	956	253	274	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Lhc2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	211	Total	C	H	N	O	S	0	0
			1663	1047	32	277	300	7		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	210	Total	C	N	O	S	0	0	0
			1609	1050	263	291	5			

- Molecule 4 is a protein called Lhc4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	211	Total	C	N	O	S	0	0	0
			1637	1058	272	303	4			

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	739	Total	C	N	O	S	0	0	0
			5799	3789	991	1001	18			

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	734	Total	C	N	O	S	0	0	0
			5813	3818	975	1007	13			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	80	Total	C	N	O	S	0	0	0
			600	370	104	115	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	142	Total	C	N	O	S	0	0	0
			1123	718	195	204	6			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	64	Total	C	N	O	0	0	0
			515	327	89	99			

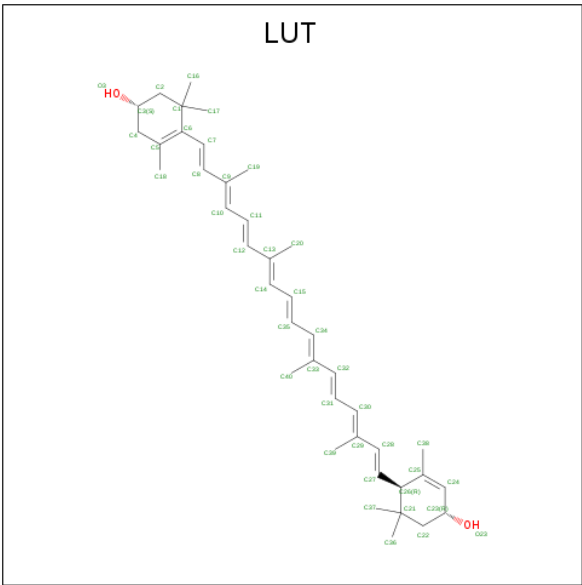
- Molecule 10 is a protein called PsaF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	163	Total	C	N	O	S	0	0	0
			1285	828	218	237	2			

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

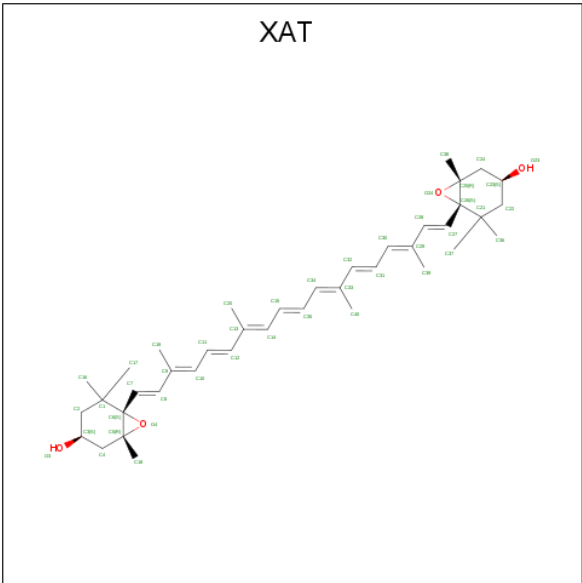
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	41	Total	C	N	O	S	0	0	0
			327	223	47	56	1			

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



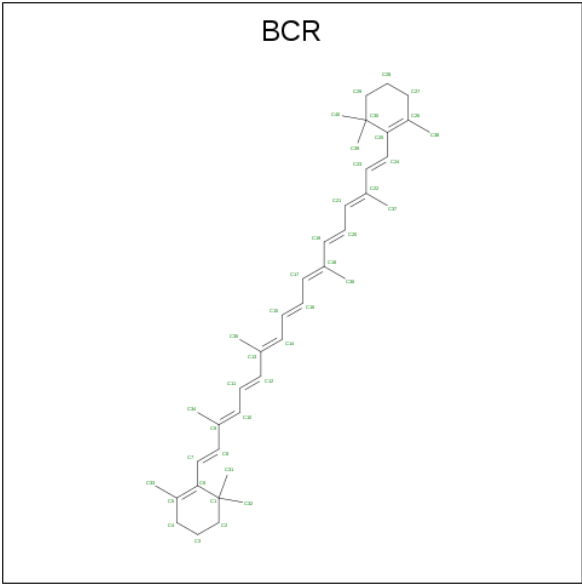
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			42	40	2		
12	2	1	Total	C	O	0	0
			42	40	2		
12	3	1	Total	C	O	0	0
			42	40	2		
12	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 13 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	1	1	Total	C	O	0	0
			44	40	4		
13	2	1	Total	C	O	0	0
			44	40	4		
13	3	1	Total	C	O	0	0
			44	40	4		
13	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



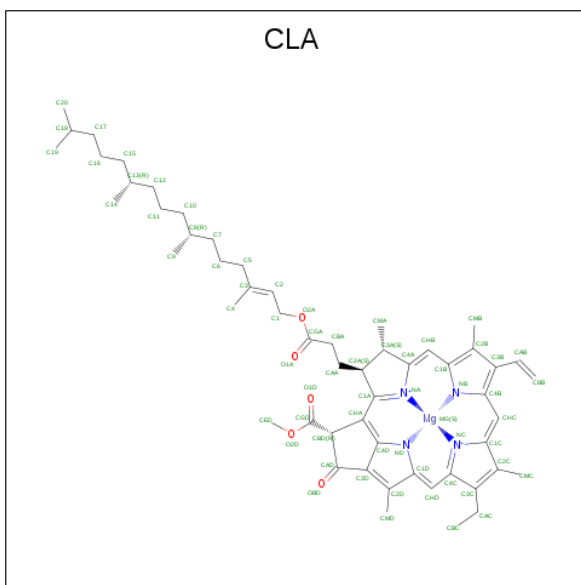
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	1	1	Total	C	0	0
			40	40		
14	1	1	Total	C	0	0
			40	40		
14	2	1	Total	C	0	0
			40	40		
14	3	1	Total	C	0	0
			40	40		
14	3	1	Total	C	0	0
			40	40		
14	4	1	Total	C	0	0
			40	40		
14	4	1	Total	C	0	0
			40	40		
14	A	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	A	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	B	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0
14	J	1	Total C 40 40	0	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	1	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	1	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	1	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	1	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
15	1	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	1	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	1	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	2	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	2	1	Total 49	C 39	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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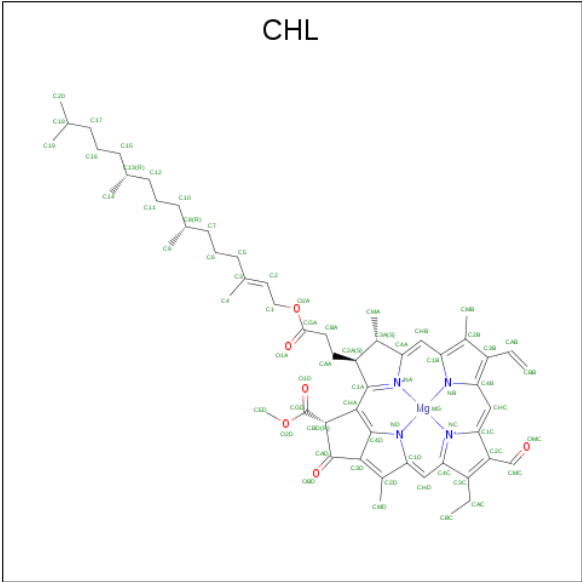
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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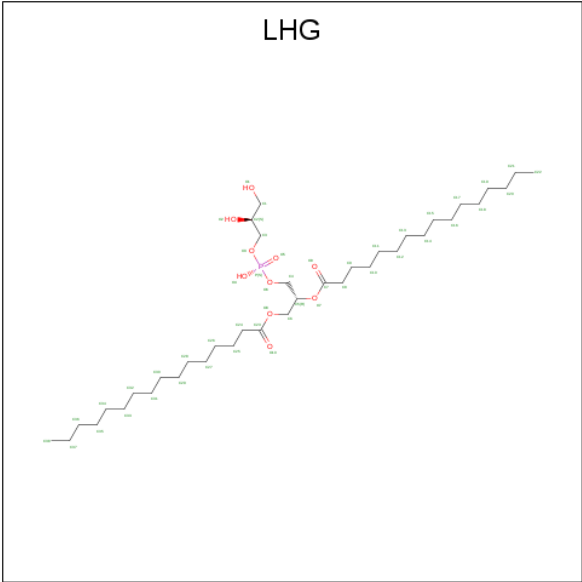
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 16 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



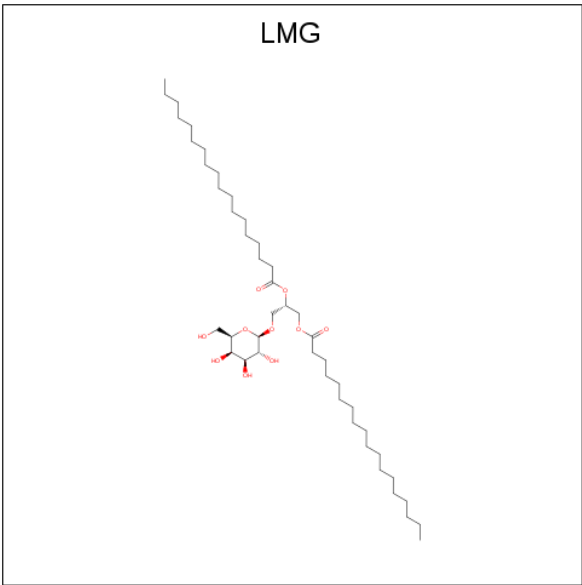
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	1	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
16	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



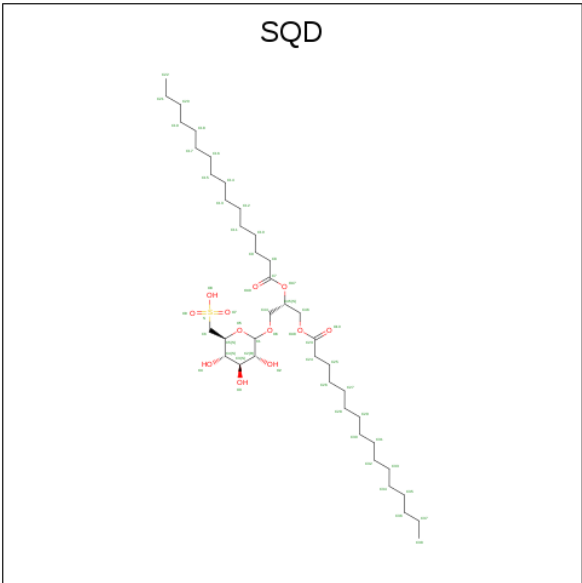
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	1	1	Total	C	O	P	0	0
			23	12	10	1		
17	2	1	Total	C	O	P	0	0
			21	10	10	1		
17	A	1	Total	C	O	P	0	0
			16	7	8	1		
17	A	1	Total	C	O	P	0	0
			24	13	10	1		
17	B	1	Total	C	O	P	0	0
			21	10	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



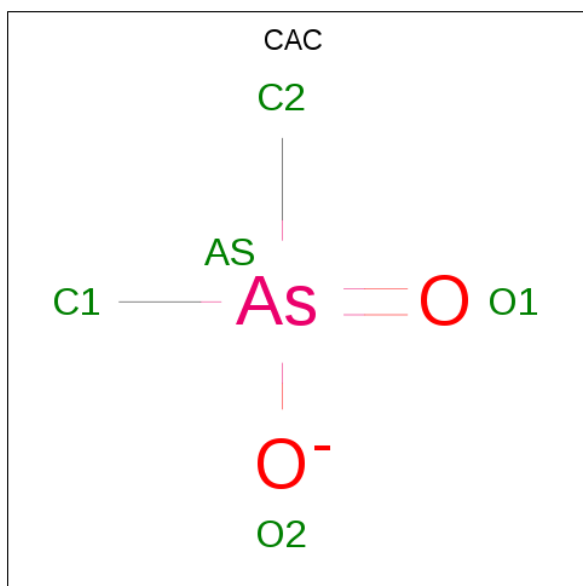
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	1	1	Total	C	O	0	0
			36	26	10		
18	1	1	Total	C	O	0	0
			23	13	10		
18	2	1	Total	C	O	0	0
			25	15	10		
18	2	1	Total	C	O	0	0
			16	9	7		

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



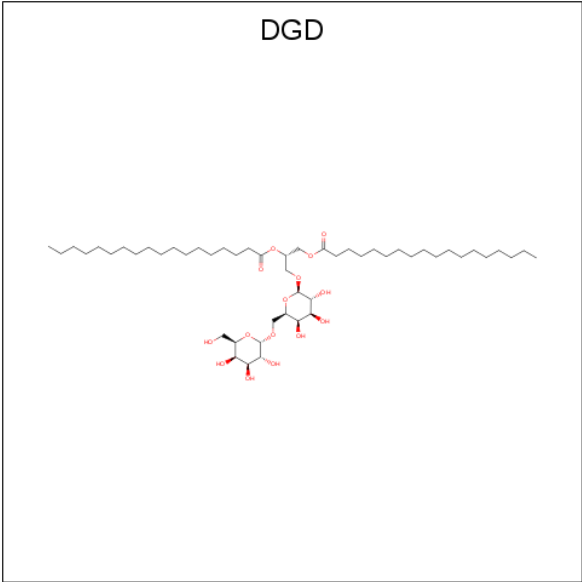
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	O	S	0	0
			40	27	12	1		

- Molecule 20 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



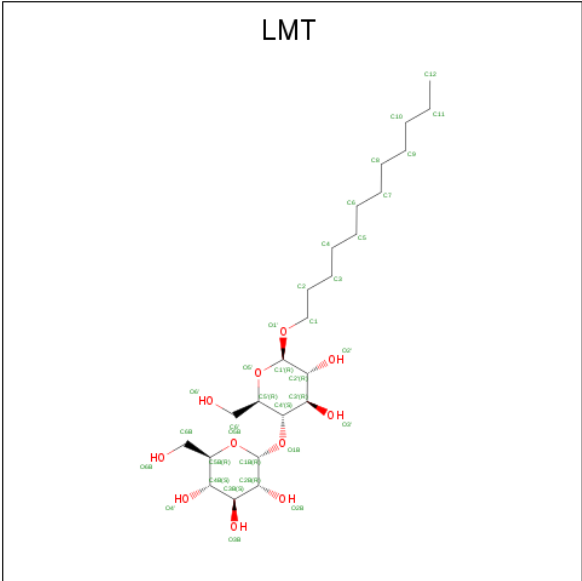
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



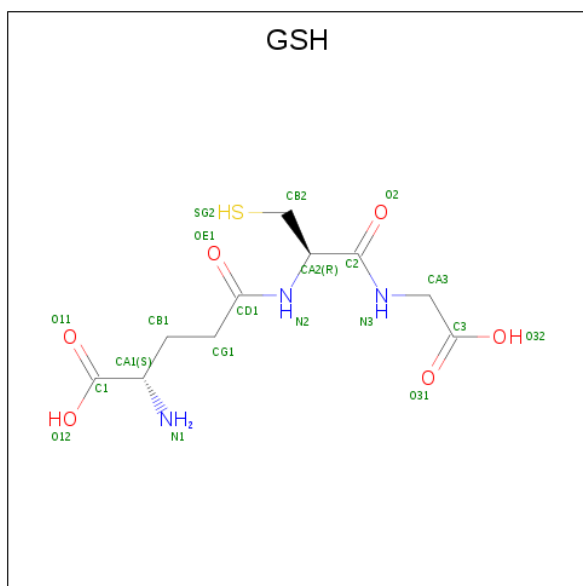
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			47	32	15		
21	4	1	Total	C	O	0	0
			45	30	15		
21	B	1	Total	C	O	0	0
			38	23	15		
21	J	1	Total	C	O	0	0
			28	15	13		

- Molecule 22 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



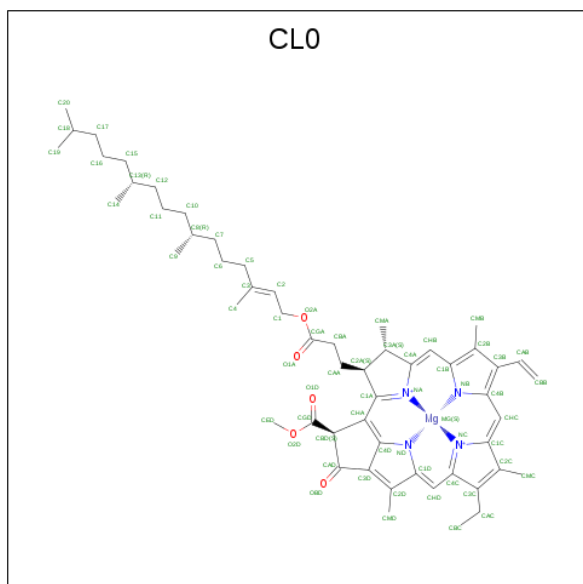
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	2	1	Total	C	O	0	0
			23	12	11		

- Molecule 23 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



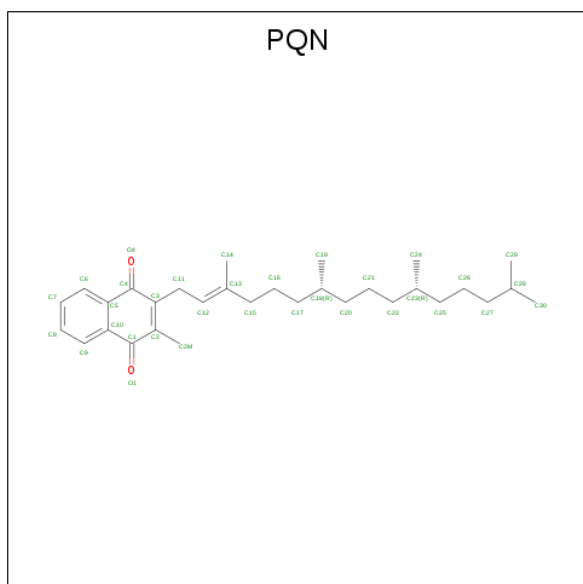
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	4	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
23	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 24 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



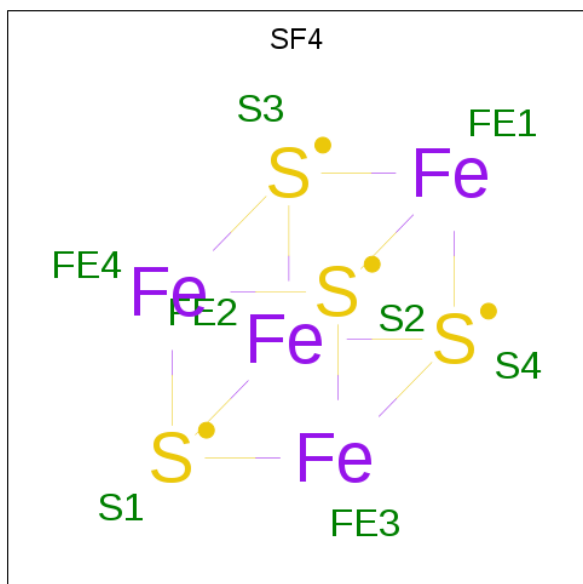
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	
			50	40	1	4	5	
							0	0

- Molecule 25 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O		
			33	31	2	0	0
25	B	1	Total	C	O		
			33	31	2	0	0

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total 8	Fe 4	S 4	0	0
26	C	1	Total 8	Fe 4	S 4	0	0
26	C	1	Total 8	Fe 4	S 4	0	0

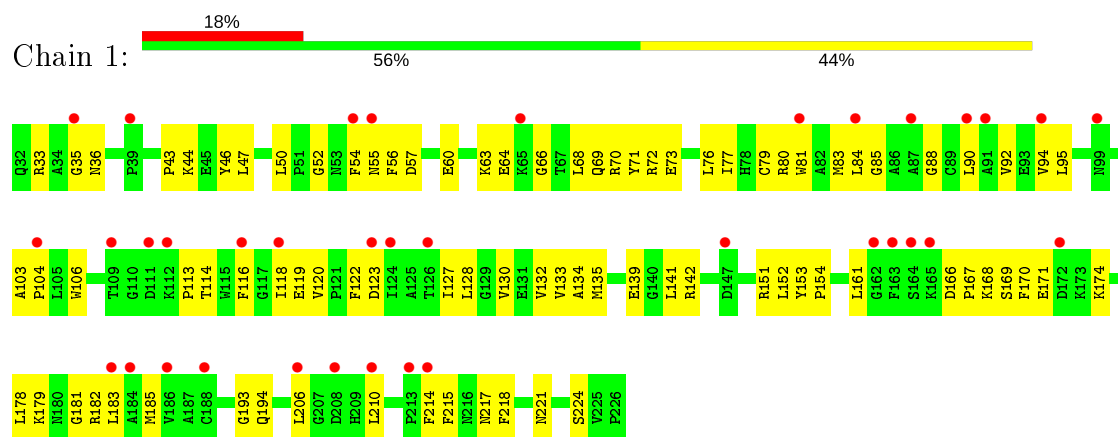
- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total 1	Ca 1	0	0

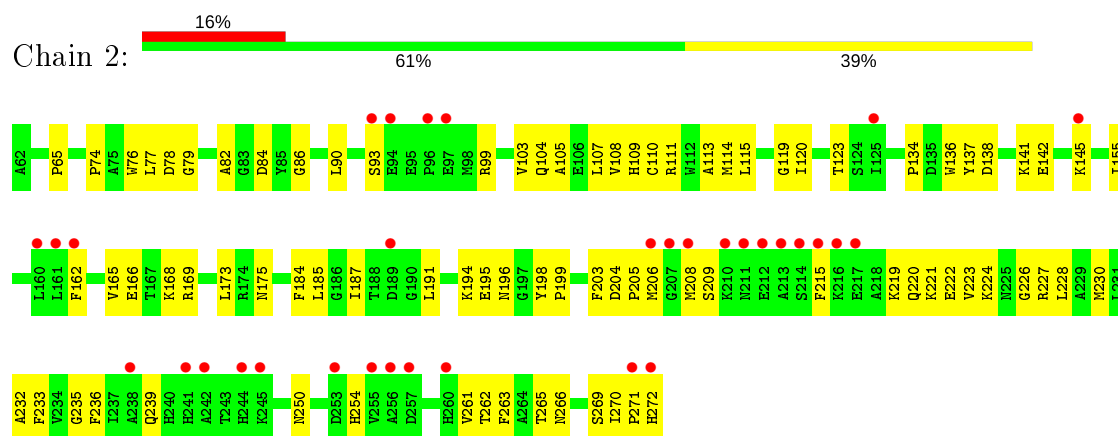
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

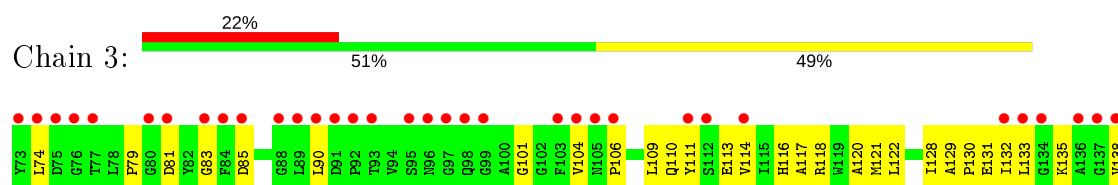
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

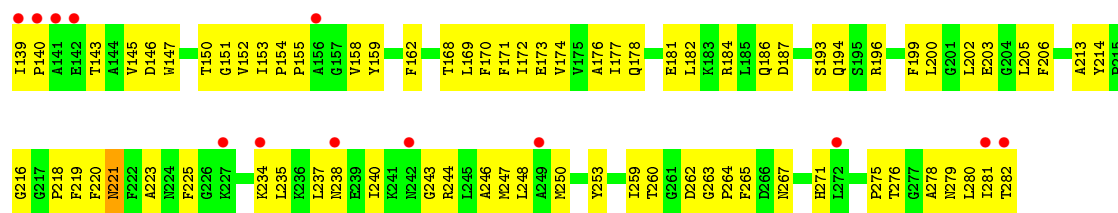


- Molecule 2: Lhc2

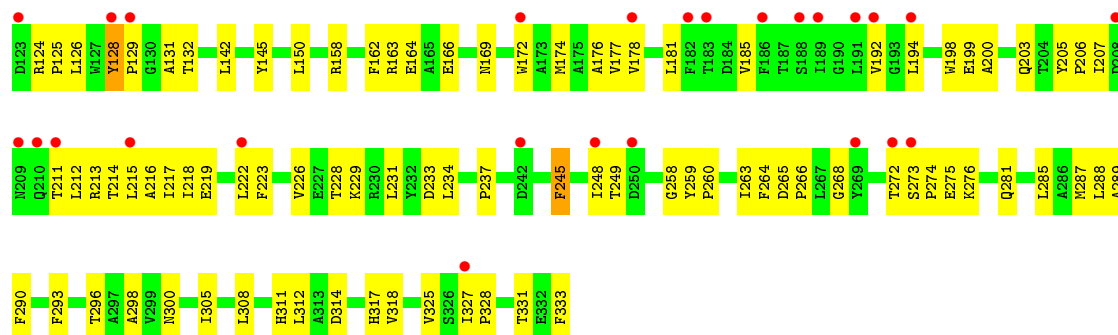


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

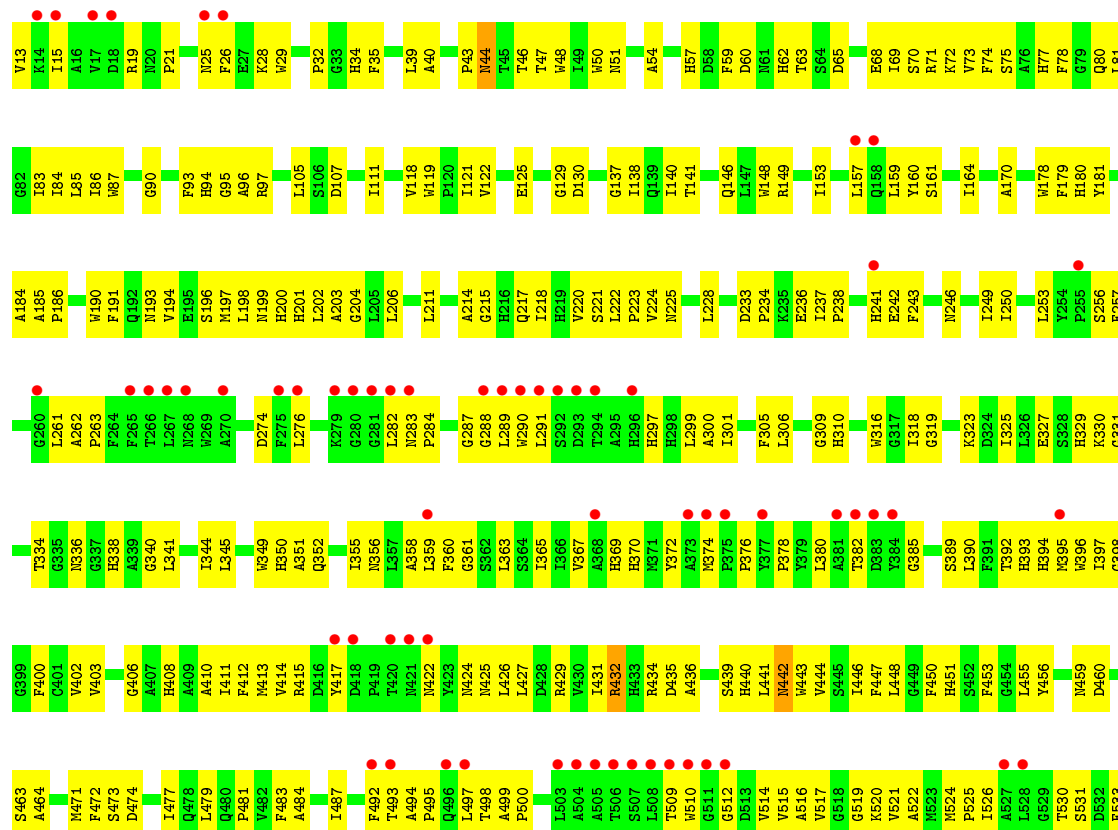


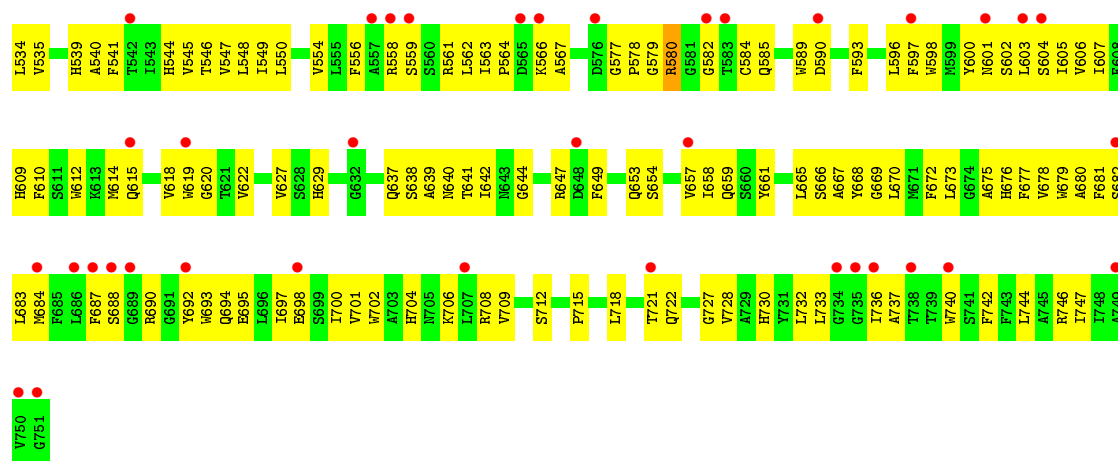


● Molecule 4: Lhc4

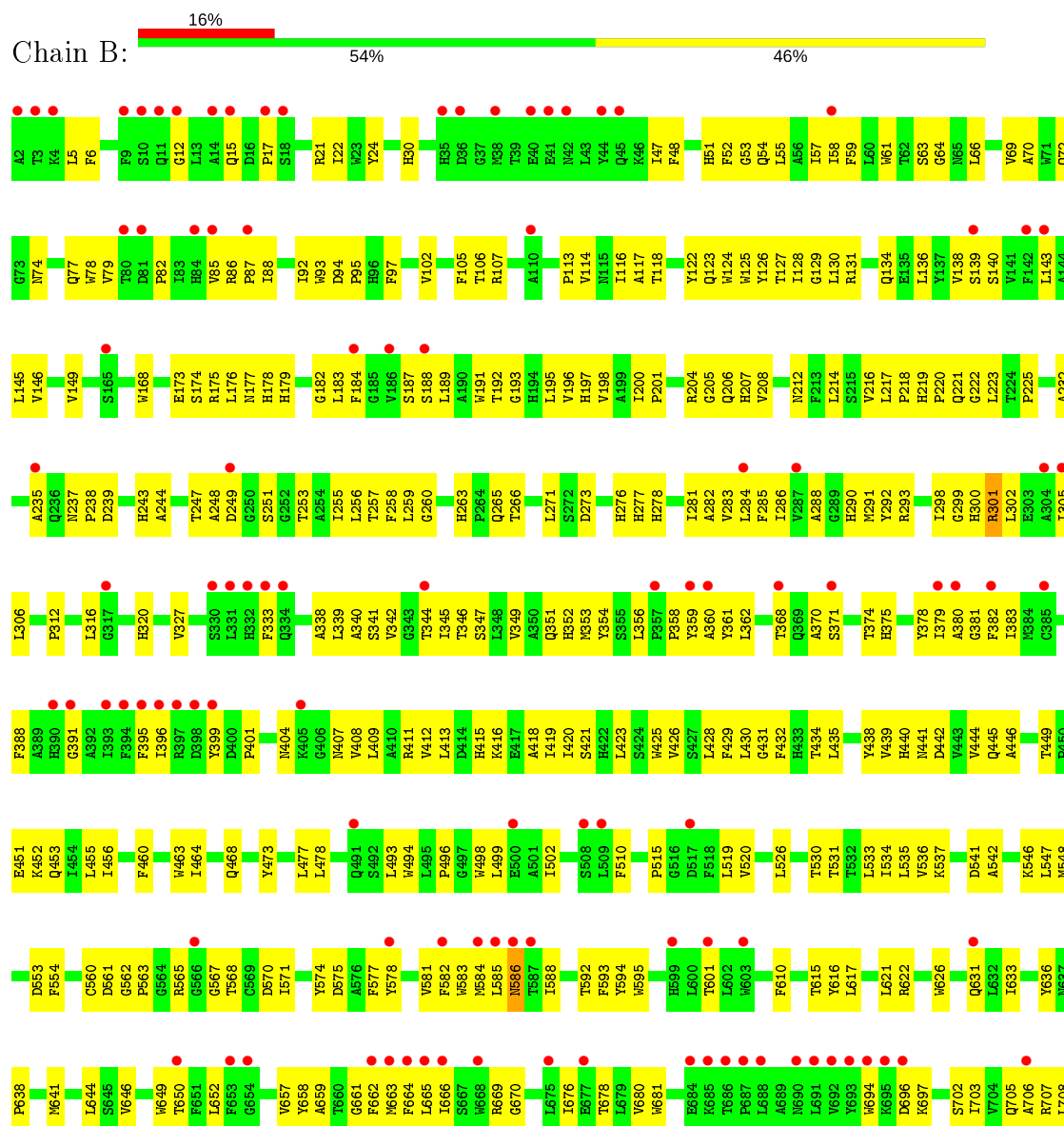


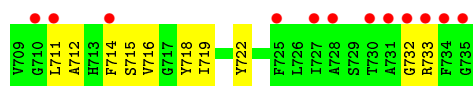
● Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



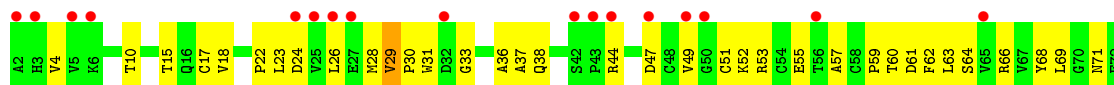


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

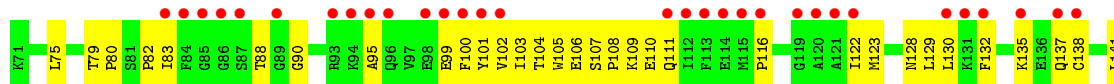




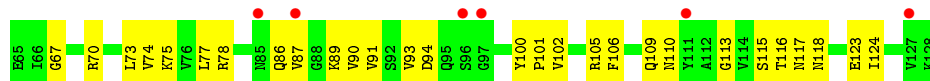
• Molecule 7: Photosystem I iron-sulfur center



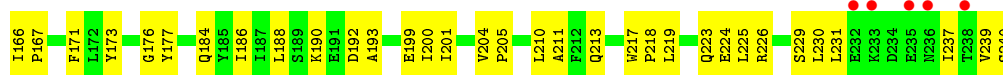
• Molecule 8: PsaD



• Molecule 9: PsaE



• Molecule 10: PsaF



• Molecule 11: Photosystem I reaction center subunit IX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	158.88Å 100.51Å 191.04Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	48.95 – 3.40 48.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-3.40) 81.3 (48.95-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.337 , 0.356 0.337 , 0.356	Depositor DCC
R_{free} test set	1593 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 4.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	30870	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LUT, DGD, XAT, LMT, SF4, CHL, CLA, PQN, CAC, GSH, LMG, CL0, CA, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.33	0/1529	0.44	0/2073
2	2	0.31	0/1680	0.43	0/2277
3	3	0.28	0/1657	0.44	0/2253
4	4	0.38	0/1687	0.47	0/2300
5	A	0.29	0/5995	0.40	0/8179
6	B	0.30	0/6026	0.40	0/8237
7	C	0.29	0/610	0.45	0/828
8	D	0.29	0/1150	0.47	0/1551
9	E	0.36	0/525	0.43	0/712
10	F	0.39	0/1313	0.45	0/1776
11	J	0.38	0/338	0.49	0/461
All	All	0.31	0/22510	0.42	0/30647

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
7	C	0	1
11	J	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	245	PHE	Peptide
7	C	29	VAL	Peptide
11	J	14	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1490	0	1457	114	1
2	2	1631	32	1575	109	0
3	3	1609	0	1567	140	0
4	4	1637	0	1579	136	0
5	A	5799	0	5629	460	0
6	B	5813	0	5565	398	0
7	C	600	0	582	48	0
8	D	1123	0	1134	77	0
9	E	515	0	508	21	0
10	F	1285	0	1304	89	0
11	J	327	0	328	43	0
12	1	42	0	55	11	0
12	2	42	0	55	12	0
12	3	42	0	55	11	0
12	4	42	0	55	18	0
13	1	44	0	56	12	0
13	2	44	0	56	15	0
13	3	44	0	56	23	0
13	4	44	0	56	5	0
14	1	80	0	105	15	0
14	2	40	0	53	8	0
14	3	80	0	105	26	0
14	4	80	0	105	12	0
14	A	240	0	318	42	0
14	B	240	0	316	34	0
14	F	40	0	52	6	0
14	J	120	0	159	26	0
15	1	593	0	468	122	0
15	2	501	0	402	66	0
15	3	525	0	391	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	4	542	0	423	95	0
15	A	2180	0	1773	325	0
15	B	2137	0	1760	280	0
15	F	96	0	72	12	0
15	J	49	0	38	8	0
16	1	97	0	66	27	0
16	2	194	0	134	31	0
16	3	47	0	30	14	0
16	4	147	0	102	21	0
17	1	23	0	16	2	0
17	2	21	0	12	2	0
17	A	40	0	30	6	0
17	B	21	0	12	2	0
18	1	59	0	58	1	0
18	2	41	0	34	1	0
19	1	40	0	46	4	0
20	1	10	0	0	0	0
20	3	10	0	0	1	0
20	4	10	0	0	1	0
21	2	47	0	52	2	0
21	4	45	0	48	7	0
21	B	38	0	34	4	0
21	J	28	0	26	0	0
22	2	23	0	21	0	0
23	4	20	0	15	0	1
23	B	20	0	15	2	0
24	A	50	0	39	23	0
25	A	33	0	46	12	0
25	B	33	0	46	6	0
26	A	8	0	0	0	0
26	C	16	0	0	2	0
27	B	1	0	0	0	0
All	All	30838	32	29094	2232	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (2232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4005:BCR:C12	14:A:4005:BCR:C11	1.83	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4005:BCR:C10	14:A:4005:BCR:C11	1.92	1.45
7:C:29:VAL:HG12	7:C:30:PRO:HD3	1.20	1.17
5:A:197:MET:HE2	15:A:1111:CLA:HAC1	1.36	1.04
8:D:105:TRP:HB3	8:D:153:PRO:HB3	1.40	1.02
6:B:5:LEU:HD13	6:B:6:PHE:H	1.24	1.02
15:A:1101:CLA:HBA2	15:A:1101:CLA:HBD	1.42	1.01
8:D:146:ARG:HH22	8:D:153:PRO:HD2	1.25	1.01
1:1:71:TYR:HB3	15:1:604:CLA:HMA1	1.43	1.00
15:A:1012:CLA:H43	6:B:439:VAL:HG22	1.41	0.99
1:1:103:ALA:HA	15:1:606:CLA:HED1	1.45	0.98
15:B:1023:CLA:HMB1	15:B:1023:CLA:HBB1	1.43	0.98
15:2:605:CLA:HAC1	15:2:612:CLA:HAA1	1.44	0.97
4:4:312:LEU:HD21	15:4:608:CLA:HMC3	1.45	0.97
1:1:217:ASN:HB3	15:1:608:CLA:HED1	1.43	0.97
14:A:4007:BCR:H363	15:B:1239:CLA:HBB1	1.47	0.96
2:2:187:ILE:HG21	2:2:191:LEU:HD13	1.47	0.96
15:A:1136:CLA:HMB1	15:A:1136:CLA:HBB1	1.47	0.96
2:2:109:HIS:HD2	15:2:612:CLA:HMD1	1.31	0.96
15:B:1230:CLA:HED1	11:J:35:ASP:HA	1.48	0.96
15:A:1128:CLA:HBB1	15:A:1128:CLA:HMB1	1.46	0.95
4:4:265:ASP:HB2	4:4:266:PRO:HD3	1.44	0.95
7:C:29:VAL:HG12	7:C:30:PRO:CD	1.96	0.95
15:A:1110:CLA:HED1	15:A:1111:CLA:HHC	1.49	0.95
15:4:601:CLA:HMB1	15:4:601:CLA:HBB1	1.49	0.95
3:3:271:HIS:HD2	3:3:275:PRO:HA	1.31	0.95
3:3:250:MET:HG2	13:3:502:XAT:H12	1.47	0.95
5:A:584:CYS:H	6:B:670:GLY:HA3	1.31	0.95
15:1:606:CLA:HBB1	15:1:606:CLA:HMB1	1.50	0.94
15:A:1013:CLA:H101	15:A:1140:CLA:HMC2	1.50	0.94
4:4:158:ARG:NH2	20:4:902:CAC:O1	2.01	0.93
3:3:155:PRO:HG3	15:A:1114:CLA:HMD2	1.50	0.93
15:J:1302:CLA:HBB1	15:J:1302:CLA:HMB1	1.51	0.93
5:A:80:GLN:HG2	15:A:1103:CLA:HMA1	1.48	0.93
16:1:610:CHL:HMC	15:1:613:CLA:HAB	1.49	0.93
15:2:601:CLA:HBB1	15:2:601:CLA:HMB1	1.49	0.93
15:A:1013:CLA:HHB	15:A:1013:CLA:H42	1.50	0.93
1:1:50:LEU:HD11	1:1:68:LEU:HD21	1.47	0.93
15:A:1108:CLA:HBD	15:A:1108:CLA:HBA1	1.51	0.92
10:F:166:ILE:HG13	10:F:167:PRO:HD3	1.48	0.92
15:B:1216:CLA:HMB1	15:B:1216:CLA:HBB1	1.48	0.92
15:A:1124:CLA:HBB1	15:A:1124:CLA:HHC	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:608:CLA:HAA2	4:4:218:ILE:HG22	1.51	0.92
3:3:259:ILE:HD11	14:3:504:BCR:H281	1.51	0.92
15:1:605:CLA:HHC	15:1:605:CLA:HBB1	1.52	0.91
7:C:17:CYS:HB3	26:C:3003:SF4:S2	2.11	0.91
15:3:606:CLA:HMB1	15:3:606:CLA:HBB1	1.53	0.91
15:3:603:CLA:HBD	15:3:603:CLA:HBA2	1.53	0.91
16:3:604:CHL:HMB1	16:3:604:CHL:HBB1	1.53	0.91
15:3:605:CLA:HBB1	15:3:605:CLA:HMB1	1.51	0.91
5:A:15:ILE:HD11	15:A:1110:CLA:HBD	1.53	0.90
15:1:603:CLA:HBD	15:1:603:CLA:HBA1	1.54	0.90
15:3:611:CLA:HMB1	15:3:611:CLA:HBB1	1.52	0.90
3:3:271:HIS:CD2	3:3:275:PRO:HA	2.08	0.89
4:4:199:GLU:OE1	4:4:203:GLN:NE2	2.06	0.89
5:A:605:ILE:HD11	24:A:1011:CL0:H35	1.55	0.88
15:A:1127:CLA:HHC	15:A:1127:CLA:HBB1	1.53	0.88
5:A:481:PRO:HD3	5:A:533:PHE:HB2	1.55	0.88
6:B:575:ASP:OD1	6:B:707:ARG:NH1	2.07	0.88
4:4:265:ASP:HB2	4:4:266:PRO:CD	2.03	0.88
5:A:70:SER:HG	5:A:349:TRP:HE1	0.90	0.88
15:A:1115:CLA:HBB1	15:A:1115:CLA:HMB1	1.55	0.88
13:3:502:XAT:H22	15:3:606:CLA:HMB3	1.55	0.87
10:F:177:TYR:HE2	15:F:1301:CLA:HBD	1.37	0.87
6:B:585:LEU:HD21	6:B:715:SER:HA	1.56	0.87
4:4:162:PHE:HB3	15:4:604:CLA:HMA1	1.57	0.87
16:3:604:CHL:HBC2	16:3:604:CHL:HHB	1.57	0.87
8:D:146:ARG:NH2	8:D:151:GLN:O	2.07	0.87
15:A:1013:CLA:HBA1	6:B:428:LEU:HD23	1.55	0.86
5:A:680:ALA:HB3	15:A:1013:CLA:HBB2	1.57	0.86
12:2:501:LUT:H361	12:2:501:LUT:H28	1.58	0.86
3:3:101:GLY:HA3	5:A:19:ARG:HD2	1.55	0.86
3:3:221:ASN:ND2	3:3:223:ALA:O	2.08	0.86
12:1:501:LUT:H371	12:1:501:LUT:H28	1.58	0.86
15:1:615:CLA:HBB1	15:1:615:CLA:HMB1	1.57	0.86
16:2:610:CHL:HMB1	16:2:610:CHL:HBB1	1.56	0.86
2:2:165:VAL:HG11	14:2:503:BCR:H16C	1.56	0.85
5:A:331:GLY:HA3	17:A:5001:LHG:HC32	1.58	0.85
15:A:1125:CLA:HBB1	15:A:1125:CLA:HHC	1.56	0.85
3:3:117:ALA:HB1	3:3:243:GLY:HA3	1.57	0.85
10:F:177:TYR:CE2	15:F:1301:CLA:HBD	2.12	0.85
3:3:151:GLY:HA3	15:3:613:CLA:HBC1	1.59	0.85
3:3:225:PHE:CD2	15:3:601:CLA:H12	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:607:CLA:HBB1	15:2:607:CLA:HMB1	1.58	0.85
24:A:1011:CL0:H15	24:A:1011:CL0:H11	1.59	0.85
6:B:64:GLY:HA3	15:B:1204:CLA:HBB1	1.59	0.85
4:4:128:TYR:HD2	4:4:132:THR:HG21	1.40	0.84
15:A:1107:CLA:HBB1	15:A:1107:CLA:HMB1	1.57	0.84
2:2:109:HIS:CD2	15:2:612:CLA:HMD1	2.12	0.84
15:A:1111:CLA:HBB1	15:A:1111:CLA:HMB1	1.59	0.84
3:3:259:ILE:HG21	15:3:603:CLA:HBA1	1.59	0.84
15:B:1227:CLA:HBB2	15:B:1236:CLA:HBB2	1.57	0.84
6:B:388:PHE:HZ	15:B:1222:CLA:HAB	1.41	0.84
12:3:501:LUT:H221	15:3:601:CLA:H2	1.59	0.84
1:1:139:GLU:OE1	1:1:142:ARG:NH2	2.11	0.83
6:B:708:LEU:HD22	21:B:5002:DGD:HB22	1.60	0.83
5:A:345:LEU:HD11	5:A:355:ILE:HD12	1.60	0.83
15:4:609:CLA:HBB1	15:4:609:CLA:HMB1	1.60	0.83
6:B:659:ALA:HB3	15:B:1023:CLA:HBB2	1.60	0.83
15:A:1012:CLA:HMA2	6:B:617:LEU:HD13	1.60	0.83
5:A:43:PRO:HG3	10:F:200:ILE:HD13	1.61	0.83
14:A:4005:BCR:C11	14:A:4005:BCR:C13	2.56	0.83
5:A:87:TRP:HA	15:A:1105:CLA:HBB2	1.59	0.83
5:A:68:GLU:HG2	5:A:72:LYS:HE2	1.61	0.82
15:B:1212:CLA:HMB1	15:B:1212:CLA:HBB1	1.58	0.82
6:B:546:LYS:HE3	10:F:237:ILE:HG22	1.61	0.82
1:1:104:PRO:HB3	15:1:613:CLA:HMC1	1.59	0.82
12:1:501:LUT:H162	15:1:608:CLA:HBC1	1.62	0.82
13:3:502:XAT:H28	13:3:502:XAT:H381	1.61	0.82
4:4:199:GLU:O	4:4:203:GLN:NE2	2.13	0.82
6:B:128:ILE:HD12	15:B:1211:CLA:HMA3	1.62	0.82
7:C:62:PHE:HB3	8:D:192:ILE:HG12	1.61	0.82
1:1:84:LEU:HG	15:1:601:CLA:HMC1	1.62	0.81
15:A:1133:CLA:H42	14:A:4005:BCR:HC7	1.61	0.81
15:4:608:CLA:HMB1	15:4:608:CLA:HBB1	1.60	0.81
3:3:205:LEU:HD23	3:3:218:PRO:HB2	1.63	0.80
15:B:1225:CLA:HBB1	15:B:1225:CLA:HHC	1.60	0.80
1:1:46:TYR:CE1	1:1:63:LYS:HG3	2.16	0.80
15:B:1239:CLA:HAC1	25:B:2002:PQN:H151	1.64	0.80
1:1:71:TYR:CB	15:1:604:CLA:HMA1	2.12	0.80
15:B:1209:CLA:HBB1	15:B:1209:CLA:HMB1	1.64	0.80
6:B:258:PHE:HD1	15:B:1214:CLA:HMB2	1.47	0.80
2:2:107:LEU:HB3	2:2:111:ARG:HH12	1.47	0.80
15:B:1022:CLA:HAC2	15:B:1023:CLA:HBC3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:284:LEU:CD1	15:B:1216:CLA:HMC1	2.11	0.80
14:A:4005:BCR:C10	14:A:4005:BCR:C12	2.59	0.80
6:B:208:VAL:HA	6:B:212:ASN:HD21	1.46	0.80
15:B:1229:CLA:HMB1	15:B:1229:CLA:HBB1	1.64	0.79
4:4:211:THR:HG23	4:4:215:LEU:HD21	1.63	0.79
15:B:1023:CLA:H3A	15:B:1023:CLA:O2A	1.82	0.79
10:F:177:TYR:OH	10:F:211:ALA:O	2.00	0.79
16:1:610:CHL:HHC	16:1:610:CHL:HBB1	1.65	0.79
15:A:1131:CLA:HHC	15:A:1131:CLA:HBB1	1.63	0.79
6:B:258:PHE:CD1	15:B:1214:CLA:HMB2	2.16	0.79
12:3:501:LUT:H28	12:3:501:LUT:H371	1.65	0.79
1:1:154:PRO:HG3	15:1:611:CLA:HMD2	1.65	0.79
5:A:463:SER:OG	5:A:471:MET:SD	2.41	0.79
5:A:75:SER:HB3	15:A:1109:CLA:HAC2	1.64	0.78
1:1:141:LEU:O	15:1:611:CLA:HBC3	1.82	0.78
1:1:221:ASN:ND2	15:1:603:CLA:OBD	2.17	0.78
15:B:1204:CLA:HMA1	15:B:1205:CLA:HMB3	1.65	0.78
15:B:1226:CLA:HBB1	15:B:1226:CLA:HMB1	1.65	0.78
15:B:1230:CLA:HBB1	15:B:1230:CLA:HMB1	1.64	0.78
15:1:606:CLA:HHH	15:1:606:CLA:HBC2	1.64	0.78
15:1:611:CLA:HBC2	15:1:611:CLA:HMC1	1.65	0.78
6:B:381:GLY:HA3	6:B:584:MET:HE2	1.65	0.78
3:3:122:LEU:HD11	14:3:503:BCR:C38	2.14	0.78
15:A:1139:CLA:HBB1	15:A:1139:CLA:HMB1	1.66	0.78
2:2:236:PHE:HE1	12:2:501:LUT:H363	1.49	0.77
5:A:687:PHE:HB2	15:A:1013:CLA:CBC	2.14	0.77
4:4:128:TYR:CD2	4:4:132:THR:HG21	2.20	0.77
5:A:43:PRO:HB3	5:A:48:TRP:CE3	2.20	0.77
14:4:505:BCR:H272	10:F:223:GLN:HE22	1.50	0.77
6:B:463:TRP:CD1	6:B:477:LEU:HD11	2.20	0.77
1:1:84:LEU:O	15:1:606:CLA:HMC3	1.84	0.77
15:A:1103:CLA:HMC3	15:A:1128:CLA:HMA1	1.67	0.77
15:A:1102:CLA:HBA2	15:A:1109:CLA:H2	1.66	0.76
7:C:10:THR:O	7:C:64:SER:OG	2.03	0.76
3:3:246:ALA:HB2	12:3:501:LUT:H202	1.67	0.76
3:3:260:THR:HG21	3:3:267:ASN:HD21	1.49	0.76
15:A:1110:CLA:HED1	15:A:1111:CLA:HAB	1.68	0.76
3:3:122:LEU:HD11	14:3:503:BCR:H383	1.65	0.76
3:3:223:ALA:HB3	15:3:601:CLA:C3	2.15	0.76
15:4:607:CLA:HMB1	15:4:607:CLA:HBB1	1.66	0.76
24:A:1011:CL0:H13	15:A:1012:CLA:OBD	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:515:PRO:HG2	10:F:147:HIS:ND1	2.00	0.76
6:B:176:LEU:HD23	6:B:292:TYR:CE2	2.21	0.76
3:3:199:PHE:CZ	14:3:503:BCR:H10C	2.20	0.76
5:A:73:VAL:HG21	15:A:1103:CLA:HBC2	1.68	0.76
4:4:174:MET:HB2	15:4:601:CLA:HMC3	1.66	0.76
11:J:9:SER:HA	11:J:13:VAL:HG21	1.65	0.76
12:1:501:LUT:H402	15:1:601:CLA:HMC2	1.68	0.75
15:1:608:CLA:HED2	15:1:608:CLA:H2A	1.68	0.75
6:B:722:TYR:HB2	15:B:1021:CLA:HED3	1.68	0.75
6:B:69:VAL:HG13	6:B:122:TYR:HE1	1.51	0.75
16:1:610:CHL:O2A	16:1:610:CHL:HBD	1.87	0.75
5:A:84:ILE:HD13	15:A:1104:CLA:HBC3	1.69	0.75
5:A:406:GLY:HA2	14:A:4005:BCR:H292	1.66	0.75
6:B:594:TYR:CE2	15:B:1234:CLA:HBC3	2.22	0.75
5:A:682:SER:HB3	5:A:730:HIS:CB	2.16	0.75
11:J:10:THR:H	11:J:13:VAL:HG22	1.49	0.75
7:C:28:MET:O	8:D:178:VAL:HG22	1.86	0.75
12:2:501:LUT:H382	15:2:608:CLA:HBC1	1.69	0.75
6:B:221:GLN:HG2	6:B:225:PRO:HD3	1.67	0.74
5:A:453:PHE:HE1	15:B:1022:CLA:HMA1	1.52	0.74
5:A:47:THR:HG22	5:A:51:ASN:OD1	1.86	0.74
6:B:358:PRO:HG3	15:B:1215:CLA:HAA2	1.70	0.74
4:4:231:LEU:HD12	15:4:612:CLA:CMA	2.17	0.74
5:A:456:TYR:HB3	5:A:642:ILE:HG13	1.68	0.74
15:1:604:CLA:H3A	15:1:604:CLA:CGA	2.18	0.74
6:B:237:ASN:ND2	6:B:253:THR:OG1	2.20	0.74
1:1:33:ARG:NH1	1:1:36:ASN:OD1	2.21	0.74
3:3:276:THR:HA	3:3:279:ASN:ND2	2.03	0.74
5:A:370:HIS:ND1	15:A:1116:CLA:OBD	2.21	0.74
6:B:5:LEU:HD13	6:B:6:PHE:N	2.00	0.74
15:2:604:CLA:HED2	15:2:604:CLA:H2A	1.68	0.73
6:B:298:ILE:HG13	6:B:299:GLY:H	1.52	0.73
15:1:604:CLA:H3A	15:1:604:CLA:O1A	1.87	0.73
6:B:223:LEU:O	6:B:223:LEU:HD13	1.86	0.73
15:1:604:CLA:HMB1	15:1:604:CLA:HBB1	1.69	0.73
13:2:502:XAT:H383	15:2:606:CLA:C2B	2.18	0.73
15:4:605:CLA:OBD	15:4:612:CLA:HBA2	1.88	0.73
3:3:199:PHE:CZ	15:3:611:CLA:HBB2	2.22	0.73
15:3:605:CLA:HMD2	15:3:612:CLA:C1D	2.19	0.73
3:3:205:LEU:CD2	3:3:218:PRO:HB2	2.18	0.73
2:2:77:LEU:HD12	2:2:77:LEU:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1113:CLA:HAB	14:A:4002:BCR:H19C	1.71	0.73
15:2:607:CLA:HBB2	14:3:503:BCR:HC7	1.71	0.72
2:2:107:LEU:HB3	2:2:111:ARG:NH1	2.04	0.72
2:2:162:PHE:HE2	16:2:613:CHL:HMB3	1.53	0.72
15:3:603:CLA:HBD	15:3:603:CLA:CBA	2.17	0.72
24:A:1011:CL0:CMB	15:A:1012:CLA:HMD1	2.20	0.72
8:D:123:MET:SD	8:D:128:ASN:ND2	2.60	0.72
2:2:166:GLU:OE1	2:2:169:ARG:NH2	2.22	0.72
15:A:1110:CLA:HBB1	15:A:1110:CLA:HMB1	1.71	0.72
6:B:595:TRP:HD1	15:B:1234:CLA:HAC1	1.54	0.72
11:J:19:ALA:HA	11:J:22:THR:OG1	1.89	0.72
1:1:217:ASN:CB	15:1:608:CLA:HED1	2.18	0.72
6:B:423:LEU:HD13	6:B:533:LEU:HA	1.71	0.72
3:3:177:ILE:HD13	14:3:503:BCR:H361	1.72	0.72
4:4:260:PRO:CG	4:4:263:ILE:HD12	2.20	0.72
6:B:578:TYR:OH	6:B:665:LEU:HD22	1.89	0.72
5:A:319:GLY:HA2	15:A:1121:CLA:HAC2	1.72	0.72
5:A:512:GLY:HA2	5:A:525:PRO:HG3	1.72	0.72
15:1:603:CLA:CB	15:1:603:CLA:HBA1	2.19	0.72
1:1:79:CYS:O	1:1:83:MET:HG3	1.90	0.72
15:B:1227:CLA:HBB2	15:B:1236:CLA:CBB	2.18	0.72
6:B:429:PHE:CE2	15:B:1235:CLA:HAB	2.25	0.72
4:4:176:ALA:HA	15:4:606:CLA:HAB	1.71	0.71
10:F:121:ALA:O	10:F:125:ARG:HD3	1.90	0.71
3:3:205:LEU:HD22	3:3:219:PHE:H	1.55	0.71
15:3:605:CLA:HMC1	15:3:605:CLA:HBC2	1.70	0.71
2:2:195:GLU:HG2	2:2:196:ASN:H	1.54	0.71
15:A:1109:CLA:HBA1	15:A:1109:CLA:CHA	2.18	0.71
1:1:218:PHE:HA	1:1:221:ASN:ND2	2.06	0.71
1:1:170:PHE:CE2	1:1:174:LYS:HD2	2.25	0.71
2:2:162:PHE:CE2	16:2:613:CHL:HMB3	2.26	0.71
6:B:577:PHE:HZ	15:B:1226:CLA:HBC3	1.54	0.71
6:B:66:LEU:HD13	6:B:139:SER:OG	1.90	0.71
15:4:602:CLA:HED1	15:4:602:CLA:H11	1.70	0.71
14:1:505:BCR:H17C	15:4:612:CLA:HMB2	1.72	0.71
2:2:168:LYS:HA	15:4:609:CLA:HED1	1.73	0.71
16:1:609:CHL:HHC	16:1:609:CHL:HBB1	1.72	0.70
15:A:1101:CLA:HBB1	15:A:1101:CLA:HMB1	1.73	0.70
6:B:657:VAL:HG11	6:B:716:VAL:HG23	1.73	0.70
6:B:570:ASP:HA	6:B:575:ASP:OD2	1.91	0.70
3:3:199:PHE:HZ	15:3:611:CLA:HBB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:PHE:CZ	4:4:217:ILE:HG21	2.27	0.70
4:4:288:LEU:CD2	15:4:604:CLA:HAC1	2.22	0.70
5:A:585:GLN:HA	5:A:590:ASP:OD2	1.92	0.70
2:2:115:LEU:HG	15:2:601:CLA:HMC1	1.73	0.70
3:3:152:VAL:HB	15:3:613:CLA:CMC	2.21	0.70
8:D:174:TYR:HB3	8:D:176:GLU:OE2	1.91	0.70
16:4:611:CHL:HHC	16:4:611:CHL:HBB1	1.73	0.70
8:D:145:LEU:HD12	8:D:153:PRO:HG3	1.73	0.70
9:E:67:GLY:HA3	9:E:93:VAL:HG11	1.72	0.70
3:3:109:LEU:HD13	16:3:604:CHL:C1	2.22	0.70
15:A:1110:CLA:HBD	15:A:1110:CLA:HBA1	1.72	0.70
6:B:371:SER:HB2	15:B:1224:CLA:HMA1	1.72	0.70
15:B:1238:CLA:HAB	25:B:2002:PQN:H171	1.73	0.70
11:J:15:GLY:H	11:J:18:TRP:HB3	1.57	0.70
15:2:602:CLA:HAB	15:2:607:CLA:HBD	1.74	0.69
15:2:608:CLA:HED2	3:3:171:PHE:CD2	2.27	0.69
12:4:501:LUT:C11	15:4:602:CLA:HMC2	2.22	0.69
5:A:605:ILE:CD1	24:A:1011:CL0:H35	2.21	0.69
6:B:562:GLY:O	6:B:568:THR:OG1	2.09	0.69
10:F:166:ILE:CG1	10:F:167:PRO:HD3	2.22	0.69
4:4:245:PHE:O	4:4:249:THR:HG23	1.91	0.69
4:4:231:LEU:HD12	15:4:612:CLA:HMA1	1.75	0.69
5:A:72:LYS:NZ	15:A:1109:CLA:OBD	2.25	0.69
16:1:610:CHL:CMC	15:1:613:CLA:HAB	2.20	0.69
2:2:162:PHE:CD2	15:2:612:CLA:HMC3	2.28	0.69
6:B:176:LEU:HD23	6:B:292:TYR:HE2	1.56	0.69
15:3:603:CLA:CBF	15:3:603:CLA:HBA2	2.22	0.69
4:4:198:TRP:O	16:4:610:CHL:HED2	1.92	0.69
13:3:502:XAT:H31	15:3:605:CLA:CMB	2.22	0.69
15:B:1229:CLA:HAB	15:B:1230:CLA:HMB2	1.72	0.69
10:F:211:ALA:HB1	15:F:1301:CLA:HED2	1.73	0.69
15:A:1108:CLA:HBA1	15:A:1108:CLA:CBF	2.22	0.69
5:A:15:ILE:HD11	15:A:1110:CLA:CBF	2.21	0.69
5:A:197:MET:CE	15:A:1111:CLA:HAC1	2.20	0.69
5:A:535:VAL:HG11	5:A:609:HIS:CD2	2.27	0.69
21:4:811:DGD:HD3	11:J:33:PHE:HE1	1.58	0.69
15:1:608:CLA:HAA2	4:4:218:ILE:CG2	2.22	0.69
6:B:54:GLN:HE22	6:B:58:ILE:HD11	1.57	0.69
1:1:135:MET:HE2	14:1:503:BCR:H362	1.73	0.69
6:B:175:ARG:HH11	15:B:1221:CLA:HMD2	1.57	0.69
15:3:603:CLA:HHC	15:3:603:CLA:HBB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1106:CLA:CHC	15:A:1107:CLA:HMD2	2.23	0.69
8:D:105:TRP:CZ3	8:D:107:SER:HB3	2.27	0.69
15:1:605:CLA:HBA1	15:1:605:CLA:H2	1.74	0.69
1:1:135:MET:HG3	15:1:612:CLA:HMC3	1.75	0.68
2:2:120:ILE:HG23	2:2:136:TRP:HB3	1.75	0.68
4:4:200:ALA:HB1	15:4:606:CLA:HED3	1.75	0.68
4:4:260:PRO:HG2	4:4:263:ILE:HD12	1.76	0.68
15:4:603:CLA:HBB1	15:4:603:CLA:HMB1	1.75	0.68
16:4:610:CHL:HHC	16:4:610:CHL:HBB1	1.75	0.68
15:B:1220:CLA:HBA2	14:B:4004:BCR:H14C	1.75	0.68
6:B:174:SER:O	6:B:178:HIS:ND1	2.25	0.68
6:B:382:PHE:O	15:B:1226:CLA:HBC2	1.93	0.68
15:A:1106:CLA:HMB1	15:A:1107:CLA:H11	1.74	0.68
5:A:178:TRP:HB2	15:A:1109:CLA:HMC3	1.72	0.68
2:2:198:TYR:HE2	2:2:219:LYS:HD2	1.57	0.68
1:1:194:GLN:HG2	15:1:603:CLA:O1D	1.93	0.68
15:A:1012:CLA:HMB3	15:B:1021:CLA:H191	1.76	0.68
15:B:1212:CLA:H2A	15:B:1212:CLA:HED2	1.75	0.68
3:3:276:THR:HA	3:3:279:ASN:HD22	1.57	0.68
15:B:1230:CLA:CED	11:J:35:ASP:HA	2.23	0.68
15:1:606:CLA:HMA2	15:1:613:CLA:HAC2	1.76	0.68
5:A:455:LEU:HD22	5:A:472:PHE:HE2	1.59	0.68
8:D:167:LEU:O	8:D:170:LYS:HG3	1.94	0.68
6:B:652:LEU:HB3	15:B:1022:CLA:H11	1.75	0.68
6:B:182:GLY:HA3	15:B:1210:CLA:HBB1	1.75	0.68
15:1:613:CLA:HBD	15:1:613:CLA:HBA1	1.76	0.68
15:B:1201:CLA:HAB	15:B:1203:CLA:CAD	2.24	0.68
2:2:113:ALA:HB2	13:2:502:XAT:H402	1.75	0.68
15:A:1138:CLA:H111	15:A:1138:CLA:HAB	1.76	0.68
5:A:516:ALA:HA	5:A:521:VAL:HA	1.75	0.68
15:A:1012:CLA:HAB	6:B:583:TRP:CH2	2.29	0.68
13:2:502:XAT:H383	15:2:606:CLA:CMB	2.24	0.67
3:3:199:PHE:N	3:3:203:GLU:OE2	2.26	0.67
15:3:605:CLA:HED2	15:3:612:CLA:O1A	1.95	0.67
15:B:1218:CLA:HMC2	15:B:1219:CLA:H12	1.76	0.67
11:J:9:SER:O	11:J:10:THR:HG23	1.94	0.67
15:2:607:CLA:HED2	15:2:607:CLA:H2A	1.74	0.67
5:A:680:ALA:C	15:A:1013:CLA:HAB	2.15	0.67
5:A:119:TRP:CH2	14:J:4002:BCR:H332	2.29	0.67
5:A:344:ILE:CD1	5:A:422:ASN:HB3	2.24	0.67
15:A:1012:CLA:HMB3	15:B:1021:CLA:H201	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:702:SER:O	6:B:706:ALA:N	2.25	0.67
9:E:110:ASN:OD1	9:E:113:GLY:N	2.28	0.67
1:1:183:LEU:HD13	15:1:607:CLA:HMD3	1.76	0.67
15:1:605:CLA:HBA1	15:1:605:CLA:C2	2.23	0.67
16:4:611:CHL:HBC2	16:4:611:CHL:HHD	1.76	0.67
6:B:423:LEU:CB	6:B:533:LEU:HD13	2.24	0.67
15:A:1012:CLA:H41	6:B:439:VAL:HG13	1.77	0.67
6:B:520:VAL:HG11	6:B:594:TYR:CD1	2.30	0.67
15:3:603:CLA:HHD	15:3:603:CLA:CBC	2.24	0.67
16:2:609:CHL:HBB1	16:2:609:CHL:HHC	1.77	0.67
3:3:259:ILE:HG21	15:3:603:CLA:CBA	2.24	0.67
4:4:178:VAL:HG22	15:4:602:CLA:CBB	2.24	0.67
2:2:239:GLN:HG2	2:2:250:ASN:ND2	2.10	0.67
15:3:603:CLA:HBD	15:3:603:CLA:CGA	2.25	0.67
4:4:264:PHE:CE2	4:4:268:GLY:HA3	2.28	0.67
2:2:104:GLN:OE1	2:2:173:LEU:HD12	1.95	0.67
2:2:262:THR:HG23	2:2:263:PHE:CD2	2.30	0.67
6:B:452:LYS:HE3	15:B:1230:CLA:HED3	1.77	0.67
14:2:503:BCR:HC42	15:4:607:CLA:CAB	2.25	0.66
5:A:687:PHE:HB2	15:A:1013:CLA:HBC1	1.76	0.66
1:1:43:PRO:HA	1:1:55:ASN:ND2	2.10	0.66
15:A:1120:CLA:HMC3	15:A:1122:CLA:HMA2	1.76	0.66
14:3:503:BCR:H292	15:3:606:CLA:NC	2.11	0.66
8:D:171:ASP:O	8:D:179:ASN:ND2	2.27	0.66
15:B:1230:CLA:HED1	11:J:35:ASP:CA	2.23	0.66
15:1:601:CLA:HMD2	15:1:611:CLA:HBA2	1.77	0.66
5:A:367:VAL:HG22	15:A:1117:CLA:H42	1.77	0.66
15:F:1302:CLA:HAB	14:F:4002:BCR:H343	1.78	0.66
12:1:501:LUT:C28	12:1:501:LUT:H371	2.25	0.66
3:3:170:PHE:O	3:3:174:VAL:HG23	1.96	0.66
5:A:584:CYS:H	6:B:670:GLY:CA	2.05	0.66
10:F:184:GLN:HG3	10:F:210:LEU:HD13	1.76	0.66
16:2:611:CHL:HHC	16:2:611:CHL:HBB1	1.76	0.66
3:3:205:LEU:HD22	3:3:219:PHE:N	2.10	0.66
8:D:197:ASP:HB3	8:D:198:PRO:HD2	1.78	0.66
6:B:271:LEU:HD13	6:B:271:LEU:O	1.94	0.66
8:D:105:TRP:HB3	8:D:153:PRO:CB	2.21	0.66
1:1:113:PRO:HG2	1:1:120:VAL:HG13	1.76	0.66
2:2:162:PHE:HD2	15:2:612:CLA:HMC3	1.61	0.66
15:4:605:CLA:HBD	15:4:605:CLA:HBA2	1.78	0.66
15:A:1124:CLA:H2	15:A:1125:CLA:HED3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:344:ILE:HD11	5:A:422:ASN:HB3	1.78	0.66
5:A:589:TRP:NE1	15:A:1128:CLA:HMD1	2.11	0.66
5:A:90:GLY:O	5:A:94:HIS:ND1	2.22	0.66
6:B:298:ILE:HG13	6:B:299:GLY:N	2.10	0.66
5:A:325:ILE:O	5:A:329:HIS:ND1	2.27	0.66
5:A:323:LYS:NZ	5:A:327:GLU:OE2	2.29	0.66
2:2:198:TYR:HA	15:2:601:CLA:CED	2.25	0.66
15:A:1102:CLA:HBB1	15:A:1102:CLA:HMB1	1.78	0.66
5:A:658:ILE:HD12	6:B:622:ARG:HG3	1.78	0.66
24:A:1011:CL0:H13	15:A:1012:CLA:HMD1	1.77	0.65
15:A:1133:CLA:HBB2	15:A:1135:CLA:H2	1.78	0.65
5:A:81:LEU:HD12	15:A:1111:CLA:HED1	1.77	0.65
16:1:609:CHL:HED1	4:4:229:LYS:HA	1.78	0.65
15:A:1013:CLA:H2	15:A:1013:CLA:H3A	1.79	0.65
5:A:580:ARG:HH12	7:C:51:CYS:HB3	1.60	0.65
16:2:609:CHL:HBA2	3:3:182:LEU:HD12	1.78	0.65
2:2:90:LEU:HD12	13:2:502:XAT:H172	1.79	0.65
14:2:503:BCR:HC42	15:4:607:CLA:HAB	1.77	0.65
15:B:1021:CLA:HMB3	15:B:1022:CLA:OBD	1.97	0.65
6:B:423:LEU:HB2	6:B:533:LEU:HD13	1.76	0.65
7:C:75:ARG:HH22	8:D:99:GLU:HG2	1.61	0.65
13:3:502:XAT:H183	15:3:606:CLA:C3B	2.26	0.65
5:A:71:ARG:HD2	5:A:185:ALA:HB1	1.77	0.65
11:J:10:THR:H	11:J:13:VAL:CG2	2.10	0.65
5:A:327:GLU:O	5:A:330:LYS:NZ	2.29	0.65
10:F:188:LEU:HD23	10:F:188:LEU:O	1.95	0.65
1:1:77:ILE:HD13	1:1:142:ARG:HH12	1.61	0.65
3:3:139:ILE:CG1	3:3:140:PRO:HD2	2.27	0.65
3:3:259:ILE:CG2	15:3:603:CLA:HBA1	2.27	0.65
5:A:215:GLY:HA3	15:A:1113:CLA:HBB1	1.77	0.65
15:A:1128:CLA:H2A	15:A:1128:CLA:HED2	1.79	0.65
5:A:178:TRP:CD1	15:A:1109:CLA:HBB1	2.31	0.65
15:A:1013:CLA:CBA	6:B:428:LEU:HD23	2.26	0.65
15:4:604:CLA:CHB	15:4:604:CLA:H2	2.27	0.65
15:A:1012:CLA:O1D	15:B:1021:CLA:H71	1.96	0.65
15:A:1105:CLA:HMB3	15:A:1106:CLA:HMA1	1.78	0.65
6:B:48:PHE:CE2	6:B:52:PHE:HE2	2.15	0.65
6:B:463:TRP:CG	15:F:1302:CLA:HMA2	2.31	0.65
10:F:139:LEU:HD12	10:F:149:ILE:HD11	1.77	0.65
15:B:1213:CLA:HBB1	15:B:1213:CLA:HMB1	1.77	0.65
1:1:35:GLY:O	1:1:54:PHE:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:610:CLA:HBB2	15:A:1114:CLA:NC	2.11	0.65
15:B:1230:CLA:H12	14:B:4006:BCR:H281	1.79	0.65
1:1:122:PHE:HE2	15:1:613:CLA:HED2	1.61	0.64
5:A:250:ILE:HD13	5:A:257:PHE:HB3	1.79	0.64
5:A:203:ALA:HB2	5:A:309:GLY:HA3	1.78	0.64
6:B:290:HIS:O	15:B:1218:CLA:HED3	1.97	0.64
5:A:718:LEU:HD22	5:A:722:GLN:NE2	2.12	0.64
8:D:146:ARG:NH2	8:D:153:PRO:HD2	2.05	0.64
5:A:374:MET:O	5:A:376:PRO:HD3	1.97	0.64
6:B:217:LEU:HD12	6:B:222:GLY:HA3	1.80	0.64
14:1:505:BCR:HC21	10:F:226:ARG:HH12	1.63	0.64
6:B:705:GLN:HG3	21:B:5002:DGD:HA22	1.80	0.64
15:1:602:CLA:O1A	15:1:602:CLA:H2A	1.97	0.64
15:2:605:CLA:CHA	15:2:605:CLA:HBA2	2.28	0.64
14:4:503:BCR:H321	14:4:503:BCR:HC8	1.78	0.64
15:A:1013:CLA:HMA1	15:A:1013:CLA:H42	1.79	0.64
3:3:154:PRO:HG2	3:3:155:PRO:HD3	1.80	0.64
3:3:177:ILE:HD13	14:3:503:BCR:C36	2.27	0.64
5:A:429:ARG:O	5:A:432:ARG:HG3	1.97	0.64
4:4:128:TYR:OH	15:4:609:CLA:HMA3	1.98	0.64
15:B:1211:CLA:HMB1	15:B:1211:CLA:HBB1	1.79	0.64
6:B:661:GLY:O	6:B:665:LEU:HG	1.98	0.64
5:A:305:PHE:HE1	15:A:1119:CLA:HAB	1.63	0.64
5:A:622:VAL:HA	5:A:627:VAL:HA	1.79	0.64
2:2:108:VAL:HG11	2:2:169:ARG:NH1	2.12	0.64
5:A:351:ALA:HB2	5:A:412:PHE:CD1	2.33	0.64
1:1:70:ARG:NH1	19:1:811:SQD:O49	2.32	0.63
5:A:359:LEU:HD11	15:A:1123:CLA:HMA1	1.79	0.63
3:3:116:HIS:HB3	3:3:247:MET:CE	2.28	0.63
14:4:505:BCR:H371	15:4:612:CLA:H12	1.80	0.63
7:C:29:VAL:CG1	7:C:30:PRO:HD3	2.14	0.63
15:2:612:CLA:HBB1	15:2:612:CLA:HMB1	1.79	0.63
15:3:603:CLA:HBD	15:3:603:CLA:O2A	1.98	0.63
15:4:605:CLA:HAC1	16:4:610:CHL:HBB2	1.79	0.63
15:B:1218:CLA:CHA	15:B:1218:CLA:HBA1	2.27	0.63
16:1:609:CHL:HAA1	4:4:228:THR:HG21	1.79	0.63
15:4:612:CLA:HED2	15:4:612:CLA:H2A	1.80	0.63
5:A:410:ALA:O	5:A:414:VAL:HG23	1.98	0.63
15:B:1202:CLA:C3	15:B:1202:CLA:HED1	2.29	0.63
3:3:280:LEU:HD22	15:3:603:CLA:NB	2.14	0.63
4:4:205:TYR:CG	4:4:206:PRO:HD3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1205:CLA:HBC2	15:B:1206:CLA:HMD2	1.80	0.63
6:B:537:LYS:NZ	6:B:541:ASP:OD2	2.32	0.63
15:A:1013:CLA:H101	15:A:1140:CLA:CMC	2.28	0.63
15:1:603:CLA:HMA1	15:1:608:CLA:HBC3	1.80	0.63
2:2:162:PHE:HZ	14:2:503:BCR:H373	1.62	0.63
16:2:613:CHL:HBB1	16:2:613:CHL:HHC	1.80	0.63
4:4:199:GLU:HA	16:4:610:CHL:HED1	1.80	0.63
3:3:247:MET:HB3	13:3:502:XAT:H402	1.79	0.63
3:3:139:ILE:HG13	3:3:140:PRO:HD2	1.80	0.63
5:A:709:VAL:HG21	15:A:1138:CLA:HMB3	1.81	0.63
15:B:1222:CLA:HAA2	15:B:1223:CLA:OBD	1.98	0.62
8:D:103:ILE:HD12	8:D:155:PHE:HE1	1.63	0.62
1:1:52:GLY:HA3	1:1:178:LEU:HD23	1.81	0.62
1:1:80:ARG:HB3	15:1:601:CLA:CBC	2.29	0.62
1:1:103:ALA:CA	15:1:606:CLA:HED1	2.27	0.62
3:3:193:SER:HA	3:3:196:ARG:HD3	1.80	0.62
15:4:606:CLA:HBB1	15:4:606:CLA:HMB1	1.80	0.62
5:A:75:SER:OG	5:A:181:TYR:HB2	1.99	0.62
5:A:647:ARG:HA	6:B:633:ILE:CG2	2.29	0.62
15:1:605:CLA:CBB	15:1:605:CLA:HHC	2.28	0.62
5:A:72:LYS:HA	15:A:1109:CLA:HMD3	1.81	0.62
6:B:79:VAL:HG13	6:B:126:TYR:CE1	2.34	0.62
3:3:260:THR:HG21	3:3:267:ASN:ND2	2.13	0.62
13:3:502:XAT:H192	15:3:606:CLA:HBB2	1.81	0.62
15:3:611:CLA:CBB	15:3:611:CLA:HMB1	2.29	0.62
4:4:288:LEU:HD23	15:4:604:CLA:HAC1	1.81	0.62
15:B:1225:CLA:HHC	15:B:1225:CLA:CBB	2.30	0.62
6:B:78:TRP:HA	6:B:85:VAL:HG11	1.81	0.62
14:1:503:BCR:H24C	15:1:613:CLA:CGA	2.29	0.62
2:2:265:THR:HG23	2:2:266:ASN:H	1.63	0.62
14:3:503:BCR:H392	15:3:613:CLA:O2A	2.00	0.62
15:4:605:CLA:H11	10:F:219:LEU:HG	1.80	0.62
15:A:1125:CLA:CBB	15:A:1125:CLA:HHC	2.29	0.62
15:B:1231:CLA:H42	15:B:1232:CLA:HBA1	1.80	0.62
10:F:192:ASP:OD1	10:F:193:ALA:N	2.33	0.62
6:B:412:VAL:HA	6:B:415:HIS:CE1	2.35	0.62
8:D:102:VAL:HG13	8:D:129:LEU:HD21	1.80	0.62
10:F:155:ALA:HA	10:F:160:HIS:HB2	1.81	0.62
4:4:314:ASP:OD2	4:4:317:HIS:ND1	2.28	0.62
15:A:1141:CLA:HMB3	17:A:5001:LHG:HC5	1.81	0.62
5:A:682:SER:HB3	5:A:730:HIS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1227:CLA:HBC1	14:B:4004:BCR:H23C	1.82	0.62
1:1:218:PHE:HZ	4:4:217:ILE:HG21	1.65	0.62
5:A:284:PRO:HA	5:A:515:VAL:HG13	1.82	0.62
6:B:255:ILE:HD12	15:B:1212:CLA:HAC2	1.81	0.62
6:B:238:PRO:HG3	6:B:259:LEU:HD11	1.82	0.62
15:A:1012:CLA:HAB	6:B:583:TRP:HH2	1.64	0.62
15:A:1101:CLA:HBA2	15:A:1101:CLA:CBD	2.25	0.62
15:A:1138:CLA:HBB1	15:A:1138:CLA:HMB1	1.81	0.62
14:A:4007:BCR:C36	15:B:1239:CLA:HBB1	2.26	0.62
7:C:61:ASP:HB3	9:E:117:ASN:ND2	2.15	0.62
1:1:77:ILE:HD13	1:1:142:ARG:NH1	2.15	0.62
5:A:119:TRP:CZ3	14:J:4002:BCR:H332	2.34	0.62
5:A:222:LEU:HB2	5:A:223:PRO:HD3	1.80	0.61
6:B:441:ASN:OD1	6:B:453:GLN:HB2	2.00	0.61
6:B:92:ILE:HG23	15:B:1206:CLA:O1D	2.00	0.61
4:4:124:ARG:HB3	4:4:125:PRO:CD	2.30	0.61
4:4:259:TYR:C	15:4:601:CLA:HED2	2.20	0.61
10:F:111:PRO:HA	10:F:116:TYR:CD2	2.35	0.61
13:1:502:XAT:H383	15:1:606:CLA:C3B	2.30	0.61
15:A:1124:CLA:CBB	15:A:1124:CLA:HHC	2.28	0.61
6:B:123:GLN:HG2	6:B:362:LEU:HA	1.81	0.61
4:4:327:ILE:HD12	15:4:615:CLA:O1D	2.01	0.61
5:A:221:SER:OG	5:A:225:ASN:OD1	2.16	0.61
5:A:345:LEU:HB2	15:A:1123:CLA:HBC3	1.81	0.61
5:A:396:TRP:CD1	15:A:1126:CLA:HAB	2.36	0.61
15:4:606:CLA:HMA2	16:4:613:CHL:HAC2	1.83	0.61
16:4:613:CHL:HBB1	16:4:613:CHL:HHC	1.82	0.61
5:A:191:PHE:HA	15:A:1111:CLA:HBC1	1.82	0.61
13:1:502:XAT:H202	15:1:604:CLA:HMC2	1.83	0.61
6:B:204:ARG:NH1	6:B:239:ASP:OD1	2.25	0.61
6:B:284:LEU:HD12	15:B:1216:CLA:HMC1	1.81	0.61
15:4:606:CLA:HMA2	16:4:613:CHL:CAC	2.31	0.61
15:A:1115:CLA:CBB	15:A:1115:CLA:HMB1	2.31	0.61
14:A:4007:BCR:H271	25:B:2002:PQN:H142	1.82	0.61
6:B:478:LEU:HD11	15:B:1232:CLA:HMC3	1.83	0.61
6:B:464:ILE:HG12	15:B:1231:CLA:HMC3	1.83	0.61
15:B:1235:CLA:HAC2	14:F:4002:BCR:HC22	1.82	0.61
15:3:601:CLA:HAC2	15:3:611:CLA:HED2	1.82	0.61
15:A:1127:CLA:HHC	15:A:1127:CLA:CBB	2.30	0.61
5:A:434:ARG:NH1	5:A:559:SER:OG	2.33	0.61
5:A:358:ALA:O	14:A:4005:BCR:H372	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:811:DGD:HG32	21:2:811:DGD:O2D	1.99	0.60
15:A:1101:CLA:CAB	14:J:4002:BCR:H271	2.31	0.60
15:A:1111:CLA:HMB1	15:A:1111:CLA:CBB	2.30	0.60
5:A:589:TRP:HE1	15:A:1128:CLA:HMD1	1.66	0.60
5:A:708:ARG:NH2	10:F:229:SER:O	2.26	0.60
1:1:183:LEU:HD21	15:1:607:CLA:HHD	1.84	0.60
13:3:502:XAT:H31	15:3:605:CLA:HMB2	1.83	0.60
15:4:607:CLA:HMB1	15:4:607:CLA:CBB	2.31	0.60
15:A:1013:CLA:O2A	6:B:428:LEU:HA	2.00	0.60
6:B:575:ASP:O	6:B:578:TYR:HB3	2.01	0.60
4:4:145:TYR:OH	4:4:281:GLN:NE2	2.34	0.60
5:A:334:THR:HG23	5:A:429:ARG:HD2	1.83	0.60
15:A:1125:CLA:HMA3	14:A:4005:BCR:H332	1.82	0.60
6:B:300:HIS:ND1	6:B:305:ILE:HD11	2.16	0.60
10:F:184:GLN:NE2	10:F:210:LEU:HD22	2.16	0.60
3:3:133:LEU:O	3:3:139:ILE:HG22	2.02	0.60
14:1:505:BCR:H372	15:4:612:CLA:H42	1.82	0.60
15:A:1133:CLA:HMD2	15:A:1134:CLA:CAB	2.31	0.60
15:A:1138:CLA:HMC1	25:A:2001:PQN:H241	1.84	0.60
5:A:580:ARG:HA	7:C:76:SER:O	2.01	0.60
5:A:666:SER:HB2	6:B:446:ALA:HB1	1.84	0.60
15:1:601:CLA:HMB1	15:1:601:CLA:HBB1	1.83	0.60
16:1:610:CHL:CHA	16:1:610:CHL:HBA2	2.31	0.60
4:4:181:LEU:O	4:4:185:VAL:HG23	2.01	0.60
15:B:1231:CLA:H61	15:B:1232:CLA:H12	1.83	0.60
13:3:502:XAT:H162	15:3:606:CLA:CMB	2.32	0.60
4:4:172:TRP:HE1	13:4:502:XAT:H191	1.67	0.60
24:A:1011:CL0:H17	24:A:1011:CL0:H23	1.82	0.60
8:D:174:TYR:O	8:D:176:GLU:N	2.35	0.60
9:E:106:PHE:O	9:E:115:SER:OG	2.18	0.60
16:1:610:CHL:CBC	15:1:613:CLA:HBC2	2.31	0.60
3:3:247:MET:HB3	13:3:502:XAT:C40	2.32	0.60
5:A:620:GLY:HA3	5:A:629:HIS:HA	1.84	0.60
4:4:245:PHE:H	4:4:249:THR:CG2	2.15	0.60
4:4:142:LEU:HD11	4:4:276:LYS:HD2	1.84	0.60
5:A:647:ARG:HA	6:B:633:ILE:HG23	1.84	0.60
6:B:378:TYR:CD2	15:B:1224:CLA:HAB	2.36	0.60
7:C:22:PRO:HD3	7:C:53:ARG:HD2	1.84	0.60
9:E:75:LYS:O	9:E:124:ILE:HG23	2.02	0.60
2:2:233:PHE:CE1	13:2:502:XAT:H30	2.36	0.60
6:B:143:LEU:HD21	14:B:4003:BCR:C40	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:536:VAL:HG22	14:B:4004:BCR:H291	1.84	0.60
12:3:501:LUT:H382	15:3:601:CLA:C1D	2.32	0.60
4:4:128:TYR:CE1	15:4:609:CLA:HMA3	2.35	0.60
15:A:1132:CLA:HHD	15:B:1206:CLA:HBB2	1.83	0.60
6:B:493:LEU:O	6:B:496:PRO:HD2	2.02	0.60
7:C:29:VAL:HG11	8:D:182:ARG:HB2	1.84	0.60
5:A:561:ARG:NH2	8:D:88:THR:O	2.35	0.60
15:1:606:CLA:CBB	15:1:606:CLA:HMB1	2.29	0.59
2:2:99:ARG:O	2:2:103:VAL:HG23	2.02	0.59
15:4:615:CLA:HBC3	21:4:811:DGD:HB31	1.82	0.59
5:A:605:ILE:HD11	24:A:1011:CL0:C4	2.31	0.59
5:A:612:TRP:HB2	5:A:649:PHE:CE1	2.36	0.59
15:B:1229:CLA:CAB	15:B:1230:CLA:HMB2	2.32	0.59
14:1:503:BCR:H24C	15:1:613:CLA:O1A	2.02	0.59
1:1:80:ARG:HB3	15:1:601:CLA:HBC2	1.85	0.59
7:C:26:LEU:H	7:C:26:LEU:HD23	1.67	0.59
10:F:184:GLN:CD	10:F:210:LEU:HD22	2.23	0.59
16:2:610:CHL:HMB1	16:2:610:CHL:CBB	2.31	0.59
13:3:502:XAT:H402	16:3:604:CHL:OMC	2.03	0.59
5:A:316:TRP:O	5:A:318:ILE:HG13	2.01	0.59
6:B:341:SER:O	6:B:345:ILE:HG12	2.02	0.59
6:B:577:PHE:CZ	15:B:1226:CLA:HBC3	2.35	0.59
8:D:100:PHE:CE1	8:D:158:VAL:HG11	2.37	0.59
2:2:187:ILE:CG2	2:2:191:LEU:HD13	2.28	0.59
2:2:198:TYR:CE2	2:2:219:LYS:HD2	2.37	0.59
12:2:501:LUT:H12	15:2:601:CLA:HAB	1.84	0.59
15:3:606:CLA:HMB1	15:3:606:CLA:CBB	2.31	0.59
12:4:501:LUT:H371	12:4:501:LUT:H28	1.83	0.59
5:A:369:HIS:HA	5:A:372:TYR:CD1	2.37	0.59
6:B:646:VAL:HG11	15:B:1205:CLA:HBC1	1.83	0.59
2:2:220:GLN:HE22	2:2:224:LYS:HE3	1.67	0.59
16:1:609:CHL:CAA	4:4:228:THR:HG21	2.32	0.59
15:A:1107:CLA:CBB	15:A:1107:CLA:HMB1	2.31	0.59
5:A:77:HIS:HB3	15:A:1111:CLA:HED2	1.84	0.59
15:A:1138:CLA:HED3	6:B:421:SER:HB2	1.83	0.59
5:A:514:VAL:HG22	5:A:524:MET:HG3	1.84	0.59
5:A:524:MET:HG3	5:A:525:PRO:HD2	1.83	0.59
6:B:388:PHE:CD2	6:B:535:LEU:HD13	2.38	0.59
6:B:657:VAL:HG22	15:B:1239:CLA:HMB3	1.83	0.59
15:1:603:CLA:HBA1	15:1:603:CLA:CHA	2.33	0.59
16:3:604:CHL:HMB1	16:3:604:CHL:CBB	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:389:SER:HB3	15:A:1126:CLA:HMA1	1.84	0.59
6:B:244:ALA:HA	6:B:265:GLN:OE1	2.03	0.59
6:B:292:TYR:CZ	6:B:302:LEU:HD21	2.37	0.59
8:D:106:GLU:HG3	8:D:108:PRO:HD3	1.85	0.59
15:1:613:CLA:HBB1	15:1:613:CLA:HMB1	1.85	0.59
5:A:157:LEU:HD23	5:A:157:LEU:O	2.02	0.59
3:3:116:HIS:HB3	3:3:247:MET:HE1	1.82	0.59
5:A:194:VAL:HG11	15:A:1123:CLA:HAC2	1.85	0.59
5:A:679:TRP:CD2	24:A:1011:CL0:H4	2.38	0.59
6:B:359:TYR:HB2	6:B:362:LEU:HD22	1.85	0.59
10:F:101:VAL:HG13	10:F:104:LYS:HE3	1.83	0.59
16:1:610:CHL:C3C	15:1:613:CLA:HMC3	2.33	0.59
3:3:111:TYR:O	3:3:114:VAL:HG22	2.03	0.59
15:A:1141:CLA:HBB1	15:A:1141:CLA:HHC	1.85	0.59
5:A:334:THR:HG21	5:A:426:LEU:HD23	1.84	0.59
5:A:682:SER:HB3	5:A:730:HIS:HB3	1.84	0.59
5:A:453:PHE:CE1	15:B:1022:CLA:HMA1	2.37	0.59
6:B:439:VAL:HG12	15:B:1230:CLA:HAC1	1.84	0.59
14:1:505:BCR:HC41	10:F:226:ARG:NH1	2.18	0.59
2:2:110:CYS:HB3	2:2:226:GLY:HA3	1.83	0.58
6:B:107:ARG:HH11	6:B:116:ILE:HG12	1.67	0.58
6:B:631:GLN:HB3	6:B:644:LEU:HD13	1.85	0.58
2:2:239:GLN:HE21	2:2:250:ASN:HB2	1.68	0.58
16:2:611:CHL:HMA2	16:2:611:CHL:HBA1	1.85	0.58
14:3:504:BCR:H341	15:3:610:CLA:HBC2	1.84	0.58
5:A:28:LYS:HB2	15:A:1109:CLA:HMA2	1.82	0.58
5:A:75:SER:O	15:A:1109:CLA:HBC1	2.02	0.58
6:B:188:SER:O	6:B:192:THR:HG23	2.03	0.58
10:F:225:LEU:HA	10:F:230:LEU:HD21	1.84	0.58
4:4:142:LEU:HD13	4:4:276:LYS:HB3	1.86	0.58
4:4:172:TRP:HH2	14:4:503:BCR:H371	1.67	0.58
5:A:160:TYR:O	5:A:164:ILE:HG12	2.03	0.58
5:A:194:VAL:HG13	15:A:1123:CLA:HHD	1.84	0.58
5:A:301:ILE:HG23	5:A:305:PHE:CE2	2.38	0.58
5:A:596:LEU:HD21	15:A:1128:CLA:HBC1	1.85	0.58
15:B:1226:CLA:HMB1	15:B:1226:CLA:CBB	2.33	0.58
6:B:143:LEU:HA	6:B:146:VAL:HG22	1.85	0.58
7:C:44:ARG:NE	8:D:167:LEU:HD11	2.19	0.58
10:F:128:ASN:HA	10:F:131:LYS:HG2	1.84	0.58
5:A:582:GLY:O	6:B:669:ARG:NH1	2.35	0.58
8:D:201:VAL:O	8:D:201:VAL:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:290:PHE:CE1	13:4:502:XAT:H8	2.39	0.58
15:A:1134:CLA:HMB1	15:A:1134:CLA:HBB1	1.85	0.58
5:A:460:ASP:OD1	5:A:641:THR:HB	2.03	0.58
5:A:697:ILE:O	5:A:701:VAL:HG23	2.04	0.58
6:B:388:PHE:CZ	15:B:1222:CLA:HAB	2.32	0.58
5:A:444:VAL:HG21	15:A:1137:CLA:HMC3	1.84	0.58
5:A:450:PHE:CE1	15:B:1023:CLA:H71	2.38	0.58
15:B:1209:CLA:HMB1	15:B:1209:CLA:CBB	2.33	0.58
5:A:396:TRP:CZ3	5:A:600:TYR:HA	2.38	0.58
15:2:608:CLA:HBB1	15:2:608:CLA:HMB1	1.85	0.58
3:3:150:THR:HG21	13:3:502:XAT:O3	2.03	0.58
3:3:282:THR:HB	15:3:603:CLA:HED2	1.84	0.58
6:B:179:HIS:HD2	6:B:183:LEU:HD22	1.68	0.58
6:B:82:PRO:HG2	6:B:361:TYR:CE2	2.38	0.58
6:B:375:HIS:O	6:B:379:ILE:HG12	2.03	0.58
8:D:108:PRO:HD2	8:D:151:GLN:NE2	2.19	0.58
15:A:1013:CLA:HMA2	15:A:1013:CLA:HBA2	1.85	0.58
6:B:196:VAL:HA	6:B:200:ILE:HD12	1.86	0.58
14:1:505:BCR:H23C	15:4:605:CLA:HMD3	1.85	0.58
12:3:501:LUT:C22	15:3:601:CLA:H2	2.32	0.58
15:A:1110:CLA:CED	15:A:1111:CLA:HAB	2.34	0.58
15:A:1139:CLA:CBB	15:A:1139:CLA:HMB1	2.34	0.58
5:A:125:GLU:OE2	10:F:125:ARG:NH2	2.32	0.58
5:A:718:LEU:HD22	5:A:722:GLN:CD	2.24	0.58
6:B:438:TYR:HE2	15:B:1021:CLA:H171	1.69	0.58
15:B:1023:CLA:HMB1	15:B:1023:CLA:CBB	2.25	0.58
15:2:607:CLA:HMB1	15:2:607:CLA:CBB	2.30	0.57
4:4:124:ARG:HB3	4:4:125:PRO:HD2	1.84	0.57
4:4:233:ASP:OD2	16:4:611:CHL:HBC1	2.03	0.57
5:A:121:ILE:HG23	5:A:122:VAL:HG22	1.85	0.57
5:A:186:PRO:HB2	5:A:191:PHE:CE2	2.38	0.57
15:A:1101:CLA:O2A	25:A:2001:PQN:H222	2.04	0.57
5:A:690:ARG:NE	5:A:718:LEU:O	2.36	0.57
15:B:1230:CLA:CBB	15:B:1230:CLA:HMB1	2.32	0.57
3:3:214:TYR:HB3	15:3:601:CLA:HED3	1.85	0.57
3:3:74:LEU:HD22	3:3:83:GLY:HA2	1.86	0.57
4:4:211:THR:O	4:4:211:THR:HG23	2.04	0.57
4:4:162:PHE:CB	15:4:604:CLA:HMA1	2.31	0.57
5:A:105:LEU:HD12	5:A:149:ARG:NH1	2.20	0.57
5:A:288:GLY:HA3	5:A:378:PRO:HA	1.84	0.57
15:B:1212:CLA:CHA	15:B:1212:CLA:HBA1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1212:CLA:HMB1	15:B:1212:CLA:CBB	2.31	0.57
15:B:1222:CLA:H2A	15:B:1222:CLA:HED2	1.86	0.57
10:F:217:TRP:CG	10:F:218:PRO:HD3	2.38	0.57
3:3:176:ALA:HB1	14:3:503:BCR:C16	2.34	0.57
13:3:502:XAT:H162	15:3:606:CLA:HMB3	1.86	0.57
5:A:524:MET:CG	5:A:525:PRO:HD2	2.34	0.57
5:A:396:TRP:HZ3	5:A:600:TYR:HA	1.68	0.57
6:B:574:TYR:OH	6:B:708:LEU:HD13	2.05	0.57
16:2:609:CHL:O2D	16:2:609:CHL:H2A	2.05	0.57
5:A:679:TRP:CZ3	5:A:683:LEU:HD11	2.39	0.57
16:1:609:CHL:CED	4:4:229:LYS:HA	2.34	0.57
1:1:95:LEU:HD13	1:1:116:PHE:HZ	1.70	0.57
2:2:220:GLN:NE2	2:2:224:LYS:HE3	2.19	0.57
15:B:1223:CLA:HMA3	14:B:4005:BCR:H312	1.86	0.57
6:B:291:MET:O	6:B:292:TYR:CG	2.57	0.57
2:2:113:ALA:HB2	13:2:502:XAT:C40	2.35	0.57
15:3:612:CLA:HAC1	15:3:613:CLA:CBB	2.34	0.57
6:B:200:ILE:HB	6:B:201:PRO:HD3	1.87	0.57
15:1:604:CLA:HMB1	15:1:604:CLA:CBB	2.34	0.57
15:1:615:CLA:CBB	15:1:615:CLA:HMB1	2.31	0.57
12:2:501:LUT:H12	15:2:601:CLA:CAB	2.34	0.57
15:A:1105:CLA:C1	15:A:1107:CLA:H42	2.34	0.57
5:A:363:LEU:O	5:A:367:VAL:HG23	2.05	0.57
5:A:441:LEU:HD23	5:A:548:LEU:HD13	1.87	0.57
5:A:677:PHE:CD2	14:A:4006:BCR:H363	2.40	0.57
6:B:351:GLN:HA	6:B:354:TYR:HE1	1.70	0.57
6:B:419:ILE:HA	15:B:1227:CLA:HBB1	1.85	0.57
2:2:145:LYS:HG2	4:4:333:PHE:HD1	1.70	0.57
4:4:248:ILE:O	4:4:248:ILE:HG22	2.03	0.57
5:A:694:GLN:O	5:A:698:GLU:HG3	2.05	0.57
15:4:608:CLA:HMB1	15:4:608:CLA:CBB	2.33	0.57
15:A:1122:CLA:HBC2	14:A:4004:BCR:HC8	1.87	0.57
5:A:736:ILE:HG21	15:A:1126:CLA:HMC2	1.85	0.57
5:A:198:LEU:HG	15:A:1123:CLA:HMD3	1.86	0.57
6:B:442:ASP:OD1	6:B:616:TYR:HB2	2.05	0.57
7:C:4:VAL:HG21	8:D:207:SER:HB2	1.86	0.57
1:1:43:PRO:HA	1:1:55:ASN:HD21	1.69	0.57
15:3:603:CLA:CBB	15:3:603:CLA:HHC	2.34	0.57
13:4:502:XAT:H183	15:4:606:CLA:C2B	2.35	0.57
15:A:1138:CLA:HMC1	25:A:2001:PQN:C24	2.35	0.57
5:A:678:VAL:HG21	5:A:733:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:82:PRO:HG2	6:B:361:TYR:CD2	2.40	0.57
6:B:66:LEU:HD23	6:B:125:TRP:CH2	2.39	0.57
6:B:581:VAL:HB	6:B:711:LEU:HD21	1.87	0.57
2:2:265:THR:HG23	2:2:266:ASN:N	2.20	0.56
15:A:1131:CLA:HHC	15:A:1131:CLA:CBB	2.33	0.56
5:A:217:GLN:HA	5:A:220:VAL:HG12	1.87	0.56
6:B:12:GLY:HA3	7:C:71:ASN:ND2	2.20	0.56
6:B:197:HIS:O	6:B:201:PRO:HG2	2.05	0.56
6:B:453:GLN:HE21	6:B:455:LEU:HD11	1.70	0.56
6:B:561:ASP:OD2	6:B:565:ARG:NH2	2.29	0.56
7:C:17:CYS:CB	26:C:3003:SF4:S2	2.83	0.56
10:F:201:ILE:HA	11:J:9:SER:O	2.04	0.56
15:2:601:CLA:HMB1	15:2:601:CLA:CBB	2.31	0.56
3:3:128:ILE:HG12	3:3:132:ILE:CD1	2.35	0.56
5:A:29:TRP:CD1	15:A:1109:CLA:H12	2.40	0.56
15:B:1216:CLA:HMB1	15:B:1216:CLA:CBB	2.29	0.56
6:B:260:GLY:HA3	6:B:494:TRP:HB2	1.87	0.56
6:B:663:MET:HB2	15:B:1023:CLA:CHC	2.35	0.56
15:A:1013:CLA:C2	15:A:1013:CLA:H3A	2.36	0.56
5:A:341:LEU:HD13	15:A:1122:CLA:HMD3	1.87	0.56
5:A:80:GLN:O	5:A:84:ILE:HG12	2.05	0.56
2:2:224:LYS:HZ2	15:2:607:CLA:CED	2.19	0.56
5:A:345:LEU:HD12	5:A:352:GLN:OE1	2.05	0.56
5:A:563:ILE:O	5:A:563:ILE:HG13	2.04	0.56
5:A:68:GLU:HA	5:A:71:ARG:HE	1.69	0.56
6:B:282:ALA:O	6:B:286:ILE:HG12	2.05	0.56
6:B:574:TYR:HE1	15:B:1226:CLA:HMD1	1.69	0.56
6:B:520:VAL:HG11	6:B:594:TYR:HB2	1.87	0.56
1:1:181:GLY:O	1:1:185:MET:HG3	2.05	0.56
15:2:607:CLA:H2A	15:2:607:CLA:CED	2.34	0.56
5:A:121:ILE:HG23	5:A:122:VAL:N	2.20	0.56
5:A:28:LYS:HE3	5:A:34:HIS:CE1	2.40	0.56
5:A:692:TYR:CE1	6:B:537:LYS:HD2	2.40	0.56
15:B:1228:CLA:HMB1	15:B:1228:CLA:HBB1	1.85	0.56
6:B:266:THR:HG22	6:B:361:TYR:CE1	2.41	0.56
6:B:257:THR:O	6:B:273:ASP:HA	2.06	0.56
15:B:1228:CLA:H2	14:F:4002:BCR:H373	1.87	0.56
15:4:615:CLA:HHC	15:4:615:CLA:HBB1	1.88	0.56
15:A:1012:CLA:CBB	6:B:526:LEU:HD21	2.35	0.56
15:A:1110:CLA:CBD	15:A:1110:CLA:HBA1	2.35	0.56
15:A:1127:CLA:CHA	15:A:1127:CLA:HBA2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:360:PHE:O	5:A:363:LEU:HG	2.06	0.56
8:D:103:ILE:HG13	8:D:154:CYS:O	2.05	0.56
6:B:473:TYR:HB3	10:F:80:ALA:HA	1.88	0.56
15:J:1302:CLA:CMC	14:J:4002:BCR:H10C	2.35	0.56
15:2:606:CLA:HBB1	15:2:606:CLA:HMB1	1.88	0.56
4:4:200:ALA:CB	15:4:606:CLA:HED3	2.36	0.56
15:A:1110:CLA:CBB	15:A:1110:CLA:HMB1	2.35	0.56
15:A:1127:CLA:H2	15:A:1127:CLA:HBA2	1.87	0.56
15:A:1137:CLA:HHC	15:A:1137:CLA:HBB1	1.88	0.56
6:B:145:LEU:O	6:B:149:VAL:HG23	2.06	0.56
15:F:1302:CLA:HBB1	15:F:1302:CLA:HMB1	1.86	0.56
15:3:603:CLA:CHA	15:3:603:CLA:HBA2	2.34	0.56
4:4:259:TYR:HB3	15:4:601:CLA:CED	2.35	0.56
6:B:340:ALA:HB2	14:B:4005:BCR:H372	1.88	0.56
6:B:644:LEU:HD11	6:B:732:GLY:HA3	1.86	0.56
2:2:105:ALA:HB2	15:2:612:CLA:HED2	1.88	0.56
5:A:121:ILE:HG13	5:A:122:VAL:HG13	1.87	0.56
5:A:670:LEU:HD13	15:A:1107:CLA:HMC1	1.87	0.56
6:B:63:SER:HB2	6:B:143:LEU:HB2	1.88	0.56
6:B:712:ALA:O	6:B:716:VAL:HG22	2.05	0.56
5:A:59:PHE:HE1	15:A:1102:CLA:HED1	1.71	0.56
5:A:204:GLY:HA2	15:A:1118:CLA:HBC1	1.87	0.56
15:B:1220:CLA:CHB	15:B:1240:CLA:HED1	2.36	0.56
6:B:59:PHE:HD1	6:B:143:LEU:HD22	1.71	0.56
7:C:73:SER:H	7:C:76:SER:HB2	1.71	0.56
8:D:155:PHE:CD2	8:D:168:HIS:HB3	2.41	0.56
15:A:1124:CLA:HBA1	15:A:1124:CLA:CHA	2.36	0.56
5:A:369:HIS:NE2	15:A:1124:CLA:OBD	2.39	0.56
15:A:1127:CLA:NC	14:A:4003:BCR:H271	2.20	0.56
5:A:385:GLY:HA2	5:A:747:ILE:HG12	1.88	0.56
6:B:520:VAL:HG11	6:B:594:TYR:CG	2.41	0.56
15:A:1124:CLA:HMB3	14:A:4005:BCR:H19C	1.88	0.55
5:A:390:LEU:HD12	5:A:394:HIS:HE1	1.70	0.55
16:3:604:CHL:HHD	16:3:604:CHL:CBC	2.34	0.55
4:4:222:LEU:HG	14:4:503:BCR:C17	2.36	0.55
15:A:1106:CLA:HED2	15:A:1106:CLA:H2A	1.87	0.55
15:A:1105:CLA:HMA1	15:A:1106:CLA:HMB3	1.87	0.55
15:A:1124:CLA:C4	15:A:1125:CLA:HED3	2.36	0.55
15:A:1124:CLA:H42	15:A:1125:CLA:HED3	1.88	0.55
5:A:224:VAL:HA	5:A:228:LEU:HD12	1.89	0.55
6:B:212:ASN:O	6:B:216:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:105:ARG:HG3	9:E:116:THR:HG22	1.89	0.55
3:3:205:LEU:HD13	3:3:219:PHE:HB2	1.88	0.55
5:A:206:LEU:HD22	15:A:1117:CLA:HMC1	1.88	0.55
5:A:456:TYR:HE1	5:A:534:LEU:HD13	1.70	0.55
5:A:597:PHE:CE1	5:A:728:VAL:HG23	2.41	0.55
15:B:1021:CLA:HBB1	15:B:1021:CLA:HMB1	1.88	0.55
6:B:72:GLN:HE22	15:B:1204:CLA:HED1	1.71	0.55
6:B:455:LEU:O	10:F:148:LEU:N	2.35	0.55
7:C:62:PHE:HE2	7:C:66:ARG:HH11	1.55	0.55
6:B:452:LYS:HD2	10:F:129:ARG:HE	1.71	0.55
3:3:132:ILE:HG12	3:3:265:PHE:CD1	2.41	0.55
5:A:211:LEU:HD23	15:A:1113:CLA:HBB2	1.88	0.55
10:F:176:GLY:HA3	10:F:217:TRP:CZ2	2.40	0.55
16:1:610:CHL:HBC2	15:1:613:CLA:HBC2	1.87	0.55
15:1:613:CLA:CB	15:1:613:CLA:HBA1	2.36	0.55
1:1:90:LEU:O	1:1:94:VAL:HG23	2.04	0.55
13:3:502:XAT:C2	15:3:606:CLA:HMB3	2.30	0.55
14:A:4006:BCR:H331	14:A:4006:BCR:C8	2.36	0.55
6:B:204:ARG:O	6:B:248:ALA:HB2	2.06	0.55
13:2:502:XAT:H383	15:2:606:CLA:HMB3	1.89	0.55
4:4:142:LEU:CD1	4:4:276:LYS:HD2	2.36	0.55
15:A:1107:CLA:CAB	15:B:1230:CLA:HMD2	2.36	0.55
5:A:68:GLU:O	5:A:72:LYS:HG3	2.07	0.55
10:F:225:LEU:HA	10:F:230:LEU:CD2	2.36	0.55
15:1:606:CLA:HMA2	15:1:613:CLA:CAC	2.35	0.55
3:3:150:THR:HG23	15:3:613:CLA:HAC2	1.89	0.55
8:D:200:LYS:O	8:D:200:LYS:HG2	2.06	0.55
1:1:214:PHE:CD1	15:1:608:CLA:HMA1	2.42	0.55
6:B:431:GLY:HA2	6:B:526:LEU:HD22	1.89	0.55
7:C:31:TRP:O	7:C:37:ALA:HB1	2.07	0.55
15:3:605:CLA:OBD	15:3:612:CLA:HBA2	2.07	0.55
4:4:260:PRO:HG3	4:4:263:ILE:HD12	1.89	0.55
5:A:34:HIS:CE1	15:A:1109:CLA:HAA1	2.41	0.55
16:2:610:CHL:HMA2	16:2:610:CHL:CGA	2.37	0.55
5:A:140:ILE:O	5:A:140:ILE:HD12	2.06	0.55
15:4:603:CLA:HMB1	15:4:603:CLA:CBB	2.37	0.54
15:A:1013:CLA:H51	6:B:432:PHE:CD1	2.43	0.54
15:A:1110:CLA:O2D	15:A:1111:CLA:HMC3	2.07	0.54
15:A:1128:CLA:CBB	15:A:1128:CLA:HMB1	2.28	0.54
15:A:1136:CLA:HBA1	15:A:1137:CLA:OBD	2.08	0.54
5:A:413:MET:O	5:A:558:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:579:GLY:C	5:A:580:ARG:HD2	2.28	0.54
6:B:358:PRO:CG	15:B:1215:CLA:HAA2	2.37	0.54
6:B:127:THR:OG1	6:B:360:ALA:N	2.39	0.54
15:B:1211:CLA:CMA	14:B:4003:BCR:H271	2.37	0.54
1:1:135:MET:CE	14:1:503:BCR:H362	2.35	0.54
4:4:308:LEU:O	4:4:312:LEU:HD23	2.08	0.54
16:4:613:CHL:O1D	16:4:613:CHL:HAA1	2.08	0.54
15:A:1108:CLA:HAB	15:A:1111:CLA:NA	2.21	0.54
14:A:4007:BCR:C27	25:B:2002:PQN:H142	2.38	0.54
5:A:336:ASN:HB3	5:A:425:ASN:ND2	2.22	0.54
6:B:277:HIS:HD2	15:B:1214:CLA:NA	2.05	0.54
2:2:82:ALA:HB1	2:2:220:GLN:HA	1.88	0.54
21:4:811:DGD:O3D	21:4:811:DGD:HG32	2.07	0.54
15:A:1013:CLA:CGA	6:B:428:LEU:HA	2.37	0.54
5:A:580:ARG:H	7:C:49:VAL:HG22	1.73	0.54
15:B:1213:CLA:HMB1	15:B:1213:CLA:CBB	2.38	0.54
6:B:291:MET:SD	15:B:1218:CLA:HMD3	2.46	0.54
6:B:530:THR:HG21	6:B:583:TRP:CE2	2.42	0.54
10:F:122:THR:HA	10:F:125:ARG:HE	1.73	0.54
15:J:1302:CLA:CBB	15:J:1302:CLA:HMB1	2.29	0.54
5:A:305:PHE:CE1	15:A:1119:CLA:HAB	2.43	0.54
5:A:510:TRP:HZ3	15:A:1125:CLA:HBC2	1.72	0.54
8:D:101:TYR:CE2	8:D:135:LYS:HB2	2.42	0.54
3:3:90:LEU:HB2	16:3:604:CHL:HBA1	1.90	0.54
4:4:164:GLU:HG3	4:4:234:LEU:HD12	1.89	0.54
14:A:4007:BCR:H383	15:B:1237:CLA:HHD	1.89	0.54
6:B:102:VAL:O	6:B:106:THR:OG1	2.22	0.54
6:B:577:PHE:CE2	15:B:1226:CLA:HMD3	2.43	0.54
10:F:105:ARG:HD2	10:F:119:LEU:HD21	1.88	0.54
5:A:589:TRP:CD1	15:A:1128:CLA:HMD1	2.42	0.54
5:A:673:LEU:O	15:A:1012:CLA:HBA1	2.08	0.54
8:D:205:THR:O	8:D:205:THR:HG22	2.07	0.54
15:A:1139:CLA:H52	11:J:14:VAL:CG2	2.37	0.54
5:A:680:ALA:CB	15:A:1013:CLA:HBB2	2.34	0.54
6:B:431:GLY:N	6:B:526:LEU:HD13	2.23	0.54
6:B:659:ALA:HB3	15:B:1023:CLA:CBB	2.36	0.54
6:B:694:TRP:CH2	6:B:697:LYS:HG2	2.42	0.54
15:A:1012:CLA:H143	14:J:4001:BCR:H14C	1.88	0.54
2:2:221:LYS:HD2	15:2:602:CLA:HMC2	1.90	0.54
15:2:612:CLA:HMB1	15:2:612:CLA:CBB	2.37	0.54
3:3:187:ASP:OD2	15:3:611:CLA:HBC1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:90:GLY:CA	15:A:1105:CLA:HMC3	2.38	0.54
15:A:1140:CLA:H91	11:J:16:LEU:HD22	1.88	0.54
5:A:688:SER:OG	5:A:693:TRP:NE1	2.36	0.54
15:A:1136:CLA:HMA1	15:A:1137:CLA:O1D	2.08	0.54
5:A:677:PHE:HB2	15:A:1012:CLA:O1A	2.08	0.54
15:B:1021:CLA:C2	15:B:1021:CLA:HBA2	2.37	0.54
6:B:434:THR:HG21	15:B:1021:CLA:H192	1.90	0.54
8:D:141:LEU:O	8:D:145:LEU:HG	2.07	0.54
2:2:199:PRO:HD2	15:2:601:CLA:HED1	1.90	0.54
15:2:608:CLA:HED2	3:3:171:PHE:HD2	1.73	0.54
2:2:77:LEU:HD11	2:2:86:GLY:HA2	1.89	0.54
5:A:59:PHE:CE1	15:A:1102:CLA:HED1	2.43	0.54
6:B:173:GLU:HA	6:B:292:TYR:CD2	2.43	0.54
8:D:110:GLU:HA	8:D:123:MET:O	2.07	0.54
4:4:285:LEU:HD21	15:4:602:CLA:HAC1	1.90	0.53
5:A:200:HIS:HB3	15:A:1111:CLA:CAB	2.36	0.53
5:A:403:VAL:HG11	5:A:596:LEU:HD23	1.89	0.53
5:A:545:VAL:O	5:A:549:ILE:HG12	2.07	0.53
6:B:266:THR:HB	6:B:361:TYR:H	1.72	0.53
7:C:36:ALA:HB1	7:C:38:GLN:OE1	2.08	0.53
1:1:103:ALA:HB3	1:1:104:PRO:HD3	1.90	0.53
1:1:183:LEU:CD1	17:1:801:LHG:HC82	2.37	0.53
16:2:613:CHL:HBD	16:2:613:CHL:HAA2	1.90	0.53
5:A:59:PHE:CD2	15:A:1103:CLA:HMC2	2.43	0.53
5:A:547:VAL:HG22	15:A:1124:CLA:HBB1	1.89	0.53
5:A:146:GLN:HG2	5:A:380:LEU:HB3	1.89	0.53
15:B:1229:CLA:HMB1	15:B:1229:CLA:CBB	2.36	0.53
8:D:104:THR:O	8:D:153:PRO:HA	2.08	0.53
16:1:609:CHL:CHA	16:1:609:CHL:HBA1	2.38	0.53
3:3:129:ALA:HB3	3:3:130:PRO:HD3	1.90	0.53
5:A:318:ILE:HA	15:A:1121:CLA:HMD3	1.90	0.53
5:A:44:ASN:O	5:A:44:ASN:ND2	2.40	0.53
6:B:105:PHE:HA	6:B:107:ARG:NH2	2.22	0.53
6:B:184:PHE:HB3	6:B:285:PHE:CD2	2.42	0.53
15:1:613:CLA:CHA	15:1:613:CLA:HBA1	2.39	0.53
4:4:177:VAL:HG13	4:4:293:PHE:CE2	2.43	0.53
15:4:601:CLA:CBB	15:4:601:CLA:HMB1	2.30	0.53
4:4:288:LEU:HD21	15:4:604:CLA:HAC1	1.89	0.53
4:4:199:GLU:HA	16:4:610:CHL:CED	2.39	0.53
21:4:811:DGD:HD3	11:J:33:PHE:CE1	2.42	0.53
15:A:1102:CLA:HMB1	15:A:1102:CLA:CBB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1124:CLA:HMB3	14:A:4005:BCR:C19	2.37	0.53
15:B:1212:CLA:NC	14:B:4001:BCR:H332	2.24	0.53
11:J:14:VAL:HA	11:J:18:TRP:H	1.72	0.53
1:1:123:ASP:O	1:1:127:ILE:HG12	2.09	0.53
3:3:79:PRO:HB2	3:3:240:ILE:HD12	1.90	0.53
5:A:441:LEU:HD23	5:A:548:LEU:CD1	2.39	0.53
5:A:450:PHE:HE1	15:B:1023:CLA:H71	1.72	0.53
6:B:106:THR:HG22	6:B:106:THR:O	2.08	0.53
6:B:66:LEU:HD12	6:B:143:LEU:HD12	1.91	0.53
8:D:204:PHE:HA	8:D:208:GLU:OE2	2.08	0.53
10:F:122:THR:HA	10:F:125:ARG:NE	2.24	0.53
10:F:225:LEU:HD12	10:F:230:LEU:HD21	1.90	0.53
11:J:10:THR:OG1	11:J:12:PRO:HD2	2.09	0.53
1:1:68:LEU:HD12	15:1:604:CLA:HMA2	1.90	0.53
15:3:605:CLA:CBB	15:3:605:CLA:HMB1	2.29	0.53
15:4:609:CLA:CBB	15:4:609:CLA:HMB1	2.34	0.53
15:A:1106:CLA:HMC3	15:A:1107:CLA:HHD	1.89	0.53
15:A:1113:CLA:HBA1	15:A:1113:CLA:CHA	2.38	0.53
5:A:39:LEU:O	5:A:48:TRP:NE1	2.41	0.53
2:2:77:LEU:HD13	2:2:84:ASP:OD1	2.09	0.53
15:3:605:CLA:HMD2	15:3:612:CLA:ND	2.23	0.53
12:4:501:LUT:C28	12:4:501:LUT:H371	2.39	0.53
9:E:73:LEU:HB3	9:E:87:VAL:CG1	2.39	0.53
1:1:52:GLY:C	15:1:604:CLA:HED1	2.29	0.53
3:3:90:LEU:HB2	16:3:604:CHL:CBA	2.38	0.53
15:A:1115:CLA:HAC2	15:A:1116:CLA:CBB	2.39	0.53
6:B:192:THR:HG22	6:B:278:HIS:HB2	1.91	0.53
2:2:198:TYR:HD2	2:2:215:PHE:HZ	1.57	0.53
4:4:169:ASN:OD1	15:4:612:CLA:HMD1	2.08	0.53
4:4:177:VAL:HG13	4:4:293:PHE:HE2	1.72	0.53
15:4:606:CLA:CBB	15:4:606:CLA:HMB1	2.39	0.53
5:A:679:TRP:CE3	24:A:1011:CL0:H4	2.44	0.53
15:A:1101:CLA:HMB1	15:A:1101:CLA:CBB	2.37	0.53
5:A:197:MET:HE2	15:A:1111:CLA:CAC	2.25	0.53
15:B:1203:CLA:HBB1	15:B:1203:CLA:HMB1	1.91	0.53
6:B:184:PHE:HD1	15:B:1215:CLA:HMC2	1.74	0.53
6:B:582:PHE:CE2	6:B:711:LEU:HD13	2.44	0.53
3:3:262:ASP:OD1	3:3:263:GLY:N	2.42	0.53
4:4:211:THR:CG2	4:4:215:LEU:HD21	2.37	0.53
15:B:1226:CLA:CAD	21:B:5002:DGD:HB32	2.39	0.53
6:B:216:VAL:O	6:B:218:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:493:LEU:HB3	6:B:494:TRP:CE3	2.44	0.53
13:1:502:XAT:H12	15:1:605:CLA:HMB2	1.91	0.52
2:2:162:PHE:CZ	14:2:503:BCR:H373	2.43	0.52
15:3:603:CLA:HHD	15:3:603:CLA:HBC2	1.90	0.52
3:3:280:LEU:O	15:3:603:CLA:HMA3	2.10	0.52
15:A:1114:CLA:HED2	15:A:1114:CLA:H2A	1.91	0.52
15:A:1115:CLA:HAC2	15:A:1116:CLA:HBB2	1.91	0.52
5:A:374:MET:SD	15:A:1125:CLA:HMC2	2.48	0.52
5:A:550:LEU:O	5:A:554:VAL:HG23	2.09	0.52
5:A:590:ASP:O	5:A:593:PHE:HB3	2.10	0.52
3:3:151:GLY:HA3	15:3:613:CLA:CBC	2.37	0.52
4:4:233:ASP:O	4:4:237:PRO:HA	2.08	0.52
15:B:1210:CLA:HBB1	15:B:1210:CLA:HMB1	1.92	0.52
15:B:1216:CLA:HMA2	15:B:1221:CLA:C1C	2.40	0.52
15:B:1229:CLA:O2A	14:B:4006:BCR:H362	2.09	0.52
13:1:502:XAT:C28	13:1:502:XAT:H381	2.38	0.52
16:1:610:CHL:HBC2	15:1:613:CLA:C2C	2.40	0.52
15:A:1110:CLA:HHD	15:A:1110:CLA:HBC2	1.91	0.52
5:A:484:ALA:HA	15:A:1135:CLA:HBA1	1.90	0.52
6:B:494:TRP:HE1	15:B:1231:CLA:CED	2.22	0.52
6:B:338:ALA:O	6:B:342:VAL:HG23	2.09	0.52
6:B:553:ASP:HB3	7:C:68:TYR:HE1	1.75	0.52
15:A:1013:CLA:C1D	6:B:583:TRP:HE1	2.21	0.52
11:J:18:TRP:CE3	11:J:19:ALA:HB2	2.45	0.52
15:3:610:CLA:HMD1	15:3:613:CLA:HAB	1.90	0.52
5:A:668:TYR:CE1	15:A:1106:CLA:HAC1	2.44	0.52
5:A:197:MET:HG2	15:A:1123:CLA:OBD	2.10	0.52
6:B:301:ARG:HD2	6:B:301:ARG:H	1.75	0.52
6:B:351:GLN:HA	6:B:354:TYR:CE1	2.45	0.52
3:3:133:LEU:CD1	3:3:138:VAL:HG21	2.39	0.52
3:3:282:THR:N	15:3:603:CLA:HED2	2.23	0.52
3:3:250:MET:HE1	13:3:502:XAT:H8	1.91	0.52
14:A:4006:BCR:H24C	15:B:1230:CLA:HMC2	1.90	0.52
6:B:396:ILE:HD11	6:B:542:ALA:HB1	1.90	0.52
8:D:194:LYS:HG3	8:D:194:LYS:O	2.10	0.52
15:1:604:CLA:O1D	15:1:604:CLA:H2A	2.10	0.52
15:1:613:CLA:CBB	15:1:613:CLA:HMB1	2.39	0.52
15:2:604:CLA:H12	15:2:604:CLA:C3A	2.38	0.52
3:3:271:HIS:HA	3:3:278:ALA:HB3	1.91	0.52
14:A:4007:BCR:H362	15:B:1023:CLA:H72	1.92	0.52
5:A:493:THR:O	5:A:497:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:700:ILE:HG22	5:A:704:HIS:CE1	2.45	0.52
6:B:187:SER:OG	15:B:1215:CLA:HAC1	2.10	0.52
6:B:391:GLY:HA2	14:B:4005:BCR:H393	1.92	0.52
6:B:561:ASP:OD1	7:C:66:ARG:NH2	2.42	0.52
1:1:73:GLU:OE2	1:1:151:ARG:NE	2.36	0.52
2:2:194:LYS:NZ	2:2:209:SER:O	2.43	0.52
13:2:502:XAT:H181	13:2:502:XAT:C8	2.39	0.52
15:4:615:CLA:HHC	15:4:615:CLA:CBB	2.39	0.52
5:A:161:SER:OG	15:A:1114:CLA:HMA2	2.10	0.52
5:A:742:PHE:CD1	24:A:1011:CL0:H27	2.45	0.52
5:A:95:GLY:HA3	5:A:148:TRP:CH2	2.45	0.52
15:B:1201:CLA:HBB1	15:B:1201:CLA:HMB1	1.92	0.52
15:B:1218:CLA:HAB	15:B:1219:CLA:CGA	2.40	0.52
6:B:256:LEU:HD11	15:B:1212:CLA:HBC1	1.92	0.52
23:B:5031:GSH:O11	23:B:5031:GSH:N2	2.43	0.52
8:D:75:LEU:CD1	8:D:102:VAL:HG11	2.40	0.52
2:2:199:PRO:HB3	16:2:611:CHL:HBC2	1.92	0.52
16:2:609:CHL:HMD2	14:3:503:BCR:H333	1.91	0.52
5:A:201:HIS:HB3	15:A:1123:CLA:HED3	1.92	0.52
5:A:370:HIS:O	5:A:374:MET:HB2	2.10	0.52
5:A:519:GLY:O	5:A:622:VAL:HG12	2.10	0.52
5:A:612:TRP:CZ3	5:A:639:ALA:HB2	2.44	0.52
6:B:340:ALA:CB	14:B:4005:BCR:H372	2.40	0.52
7:C:24:ASP:O	7:C:44:ARG:NH2	2.43	0.52
7:C:29:VAL:CG1	7:C:30:PRO:CD	2.80	0.52
14:B:4006:BCR:H372	10:F:171:PHE:CD1	2.45	0.52
10:F:83:THR:HG23	10:F:84:PRO:HD2	1.92	0.52
15:2:603:CLA:HHC	15:2:603:CLA:HBB1	1.91	0.52
3:3:259:ILE:HD13	15:3:603:CLA:HAA2	1.92	0.52
15:A:1137:CLA:HHC	15:A:1137:CLA:CBB	2.40	0.52
15:A:1141:CLA:CBB	15:A:1141:CLA:HHC	2.39	0.52
5:A:443:TRP:CD2	15:A:1130:CLA:HAB	2.45	0.52
5:A:77:HIS:C	15:A:1111:CLA:HED2	2.30	0.52
6:B:664:PHE:CE1	15:B:1239:CLA:HBC3	2.45	0.52
8:D:102:VAL:HB	8:D:156:TYR:HB2	1.91	0.52
1:1:44:LYS:HB3	1:1:46:TYR:CD2	2.45	0.51
2:2:103:VAL:O	2:2:107:LEU:HG	2.10	0.51
3:3:216:GLY:N	15:3:601:CLA:HED2	2.24	0.51
4:4:223:PHE:CZ	15:4:612:CLA:HBC2	2.45	0.51
5:A:60:ASP:OD2	5:A:350:HIS:NE2	2.43	0.51
5:A:612:TRP:HZ3	5:A:639:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:143:LEU:HD11	14:B:4003:BCR:H401	1.91	0.51
2:2:175:ASN:HB3	4:4:131:ALA:HB2	1.91	0.51
5:A:238:PRO:HB2	5:A:243:PHE:CE1	2.45	0.51
5:A:556:PHE:O	5:A:566:LYS:NZ	2.23	0.51
6:B:658:TYR:CE2	15:B:1021:CLA:HMA1	2.45	0.51
6:B:15:GLN:O	6:B:17:PRO:HD3	2.09	0.51
13:1:502:XAT:H202	15:1:604:CLA:CMC	2.40	0.51
5:A:679:TRP:CD2	24:A:1011:CL0:CMA	2.93	0.51
5:A:330:LYS:HE3	5:A:336:ASN:HA	1.92	0.51
5:A:336:ASN:HB3	5:A:425:ASN:HD22	1.76	0.51
5:A:439:SER:HB3	6:B:678:THR:HG22	1.91	0.51
5:A:545:VAL:HG11	5:A:598:TRP:CH2	2.45	0.51
6:B:396:ILE:CD1	6:B:542:ALA:HB1	2.41	0.51
6:B:588:ILE:O	6:B:592:THR:HG23	2.10	0.51
8:D:110:GLU:HG3	8:D:123:MET:O	2.10	0.51
4:4:259:TYR:HB3	15:4:601:CLA:HED3	1.92	0.51
5:A:107:ASP:HB3	5:A:111:ILE:HD12	1.91	0.51
5:A:345:LEU:HD11	5:A:355:ILE:CD1	2.38	0.51
6:B:105:PHE:HA	6:B:107:ARG:HH21	1.75	0.51
15:B:1202:CLA:HED2	15:B:1221:CLA:HBA1	1.91	0.51
15:B:1221:CLA:HMB1	15:B:1221:CLA:HBB1	1.93	0.51
6:B:204:ARG:HG3	6:B:251:SER:HB2	1.92	0.51
6:B:259:LEU:O	6:B:494:TRP:HA	2.11	0.51
6:B:47:ILE:HG22	6:B:51:HIS:CE1	2.45	0.51
8:D:101:TYR:HE2	8:D:135:LYS:HB2	1.74	0.51
8:D:190:ARG:HH22	8:D:210:PHE:HB2	1.76	0.51
1:1:161:LEU:HD12	12:1:501:LUT:H222	1.92	0.51
2:2:114:MET:HB3	12:2:501:LUT:C15	2.41	0.51
13:2:502:XAT:H41	15:2:604:CLA:O1A	2.10	0.51
5:A:709:VAL:HG22	5:A:709:VAL:O	2.11	0.51
6:B:438:TYR:CE1	6:B:519:LEU:HD13	2.45	0.51
6:B:676:ILE:O	6:B:680:VAL:HG23	2.11	0.51
7:C:57:ALA:O	7:C:59:PRO:HD3	2.11	0.51
8:D:111:GLN:O	8:D:122:ILE:HD12	2.11	0.51
14:J:4001:BCR:HC8	14:J:4001:BCR:H311	1.91	0.51
15:1:607:CLA:CBB	14:4:503:BCR:H333	2.41	0.51
15:4:603:CLA:CHB	15:4:608:CLA:HMD3	2.41	0.51
5:A:395:MET:HB3	5:A:603:LEU:HD12	1.93	0.51
15:B:1211:CLA:CBB	15:B:1211:CLA:HMB1	2.39	0.51
10:F:114:ALA:HB3	10:F:115:PRO:HD3	1.93	0.51
15:1:606:CLA:HBC2	15:1:606:CLA:CHD	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:610:CHL:C2C	15:1:613:CLA:HMC3	2.41	0.51
2:2:239:GLN:HG2	2:2:250:ASN:HD22	1.74	0.51
2:2:168:LYS:CA	15:4:609:CLA:HED1	2.39	0.51
15:A:1138:CLA:CBB	15:A:1138:CLA:HMB1	2.40	0.51
5:A:220:VAL:HG22	5:A:220:VAL:O	2.10	0.51
5:A:369:HIS:HA	5:A:372:TYR:HD1	1.74	0.51
5:A:509:THR:O	5:A:526:ILE:N	2.37	0.51
5:A:83:ILE:O	5:A:86:ILE:HG22	2.10	0.51
6:B:72:GLN:HE22	15:B:1204:CLA:CED	2.24	0.51
1:1:106:TRP:CE2	1:1:113:PRO:HB3	2.45	0.51
1:1:88:GLY:O	1:1:92:VAL:HG23	2.11	0.51
15:A:1136:CLA:HMB1	15:A:1136:CLA:CBB	2.29	0.51
6:B:177:ASN:OD1	6:B:292:TYR:HB2	2.10	0.51
15:1:601:CLA:CBB	15:1:601:CLA:HMB1	2.41	0.51
16:2:609:CHL:H11	3:3:178:GLN:HE21	1.75	0.51
16:2:609:CHL:HHD	16:2:609:CHL:HBC2	1.92	0.51
3:3:118:ARG:HH12	15:3:601:CLA:C1D	2.22	0.51
5:A:740:TRP:HD1	15:A:1126:CLA:HMB2	1.76	0.51
5:A:233:ASP:CG	5:A:234:PRO:HD2	2.32	0.51
5:A:85:LEU:HB2	5:A:170:ALA:HB2	1.92	0.51
6:B:356:LEU:HD13	15:B:1214:CLA:HAA1	1.93	0.51
11:J:9:SER:CA	11:J:13:VAL:HG21	2.37	0.51
4:4:192:VAL:CG1	4:4:194:LEU:HG	2.41	0.51
15:A:1116:CLA:O1D	15:A:1117:CLA:HHB	2.11	0.51
6:B:703:ILE:HG22	6:B:707:ARG:HH21	1.76	0.51
9:E:86:GLN:NE2	10:F:237:ILE:HD11	2.25	0.51
14:2:503:BCR:H271	15:2:606:CLA:C1B	2.40	0.50
15:2:605:CLA:OBD	15:2:605:CLA:H8	2.10	0.50
4:4:128:TYR:CZ	15:4:609:CLA:HMA3	2.47	0.50
5:A:601:ASN:OD1	24:A:1011:CL0:H36	2.11	0.50
5:A:29:TRP:NE1	15:A:1109:CLA:O1A	2.43	0.50
15:B:1021:CLA:CBB	15:B:1021:CLA:HMB1	2.42	0.50
6:B:595:TRP:CD1	15:B:1234:CLA:HAC1	2.42	0.50
7:C:75:ARG:HH12	8:D:99:GLU:HG2	1.76	0.50
3:3:152:VAL:HB	15:3:613:CLA:HMC1	1.93	0.50
15:4:602:CLA:HBB1	15:4:602:CLA:HMB1	1.94	0.50
5:A:477:ILE:O	5:A:477:ILE:HG23	2.11	0.50
6:B:425:TRP:CH2	15:B:1228:CLA:HAB	2.45	0.50
3:3:154:PRO:N	3:3:155:PRO:CD	2.74	0.50
15:4:605:CLA:HMD2	15:4:612:CLA:C1D	2.41	0.50
5:A:400:PHE:O	15:A:1128:CLA:HMC1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1228:CLA:HMB1	15:B:1228:CLA:CBB	2.41	0.50
6:B:468:GLN:HG3	6:B:510:PHE:CE2	2.46	0.50
6:B:430:LEU:HB3	6:B:526:LEU:HB2	1.92	0.50
7:C:18:VAL:HG22	7:C:26:LEU:HG	1.93	0.50
1:1:183:LEU:HD12	17:1:801:LHG:HC82	1.94	0.50
2:2:228:LEU:HD23	15:2:602:CLA:HAA1	1.93	0.50
3:3:159:TYR:HB3	3:3:162:PHE:CE2	2.47	0.50
5:A:206:LEU:HD22	15:A:1117:CLA:CMC	2.41	0.50
15:B:1220:CLA:H2A	15:B:1220:CLA:O2D	2.12	0.50
15:A:1013:CLA:H51	6:B:432:PHE:CE1	2.46	0.50
8:D:188:ASN:HD21	8:D:211:GLU:HB3	1.76	0.50
1:1:95:LEU:HD13	1:1:116:PHE:CZ	2.47	0.50
15:2:602:CLA:H2	15:2:602:CLA:O1D	2.10	0.50
15:3:601:CLA:HHD	15:3:601:CLA:HBC2	1.94	0.50
15:A:1012:CLA:HMB1	15:A:1012:CLA:HBB1	1.93	0.50
15:A:1108:CLA:CED	15:A:1108:CLA:H2A	2.41	0.50
5:A:499:ALA:HB1	15:A:1134:CLA:HED1	1.94	0.50
5:A:83:ILE:HA	5:A:86:ILE:HG22	1.92	0.50
6:B:290:HIS:CE1	14:B:4001:BCR:H363	2.47	0.50
6:B:662:PHE:HD2	15:B:1022:CLA:HMD2	1.76	0.50
5:A:712:SER:N	10:F:199:GLU:OE2	2.31	0.50
1:1:54:PHE:HZ	1:1:179:LYS:HE2	1.77	0.50
3:3:106:PRO:O	3:3:110:GLN:HG2	2.12	0.50
4:4:259:TYR:CA	15:4:601:CLA:HED2	2.42	0.50
3:3:101:GLY:HA3	5:A:19:ARG:NH1	2.27	0.50
5:A:340:GLY:N	5:A:424:ASN:OD1	2.30	0.50
5:A:96:ALA:HB2	5:A:159:LEU:HB3	1.92	0.50
6:B:299:GLY:O	15:B:1218:CLA:HMA3	2.11	0.50
6:B:530:THR:HG21	6:B:583:TRP:CZ2	2.46	0.50
6:B:92:ILE:HG21	6:B:97:PHE:CE2	2.47	0.50
7:C:15:THR:HG22	7:C:28:MET:CE	2.41	0.50
11:J:27:ILE:HG21	14:J:4002:BCR:H343	1.94	0.50
3:3:170:PHE:O	3:3:173:GLU:HG2	2.11	0.50
3:3:169:LEU:HD13	15:3:613:CLA:HMD3	1.94	0.50
4:4:158:ARG:HE	10:F:223:GLN:HG3	1.77	0.50
25:A:2001:PQN:H161	14:B:4006:BCR:H333	1.92	0.50
5:A:340:GLY:O	5:A:344:ILE:HG12	2.12	0.50
6:B:441:ASN:HB3	6:B:616:TYR:HB3	1.93	0.50
8:D:181:GLY:O	8:D:182:ARG:HD2	2.12	0.50
10:F:161:ALA:O	10:F:165:PHE:HB3	2.11	0.50
14:J:4001:BCR:H321	14:J:4001:BCR:C8	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:PHE:HE1	15:1:608:CLA:O1D	1.93	0.50
2:2:261:VAL:HG22	2:2:262:THR:N	2.26	0.50
15:3:603:CLA:HHD	15:3:603:CLA:HBC3	1.92	0.50
24:A:1011:CL0:O1A	15:B:1022:CLA:HMD3	2.11	0.50
15:A:1129:CLA:HMB1	15:A:1129:CLA:HBB1	1.93	0.50
5:A:287:GLY:HA2	5:A:517:VAL:HG21	1.93	0.50
5:A:141:THR:HG21	5:A:744:LEU:HD11	1.93	0.50
7:C:79:LEU:HD22	7:C:81:TYR:CZ	2.47	0.50
11:J:16:LEU:O	11:J:20:ILE:HG12	2.11	0.50
15:2:608:CLA:CBB	15:2:608:CLA:HMB1	2.41	0.50
5:A:564:PRO:HB3	8:D:116:PRO:HB2	1.94	0.50
5:A:647:ARG:NH1	6:B:638:PRO:HD3	2.27	0.50
6:B:464:ILE:O	6:B:468:GLN:HG2	2.12	0.50
10:F:106:LEU:HD13	10:F:119:LEU:HB3	1.93	0.50
15:F:1302:CLA:HMB1	15:F:1302:CLA:CBB	2.42	0.50
15:2:603:CLA:HHC	15:2:603:CLA:CBB	2.42	0.49
21:2:811:DGD:HA32	21:2:811:DGD:O2G	2.12	0.49
4:4:287:MET:SD	15:4:604:CLA:HBB1	2.52	0.49
4:4:289:ALA:HB2	12:4:501:LUT:C10	2.42	0.49
15:A:1107:CLA:HMA1	11:J:27:ILE:HD13	1.93	0.49
15:A:1116:CLA:O1D	15:A:1117:CLA:HMA1	2.12	0.49
15:A:1134:CLA:CBB	15:A:1134:CLA:HMB1	2.41	0.49
5:A:202:LEU:HA	5:A:206:LEU:HD12	1.94	0.49
15:B:1204:CLA:HMA1	15:B:1205:CLA:CMB	2.39	0.49
6:B:425:TRP:CZ2	15:B:1228:CLA:HAB	2.47	0.49
10:F:166:ILE:HD11	11:J:39:PHE:HB2	1.92	0.49
15:1:606:CLA:HMA1	15:1:613:CLA:C2C	2.42	0.49
1:1:127:ILE:HD12	15:1:613:CLA:C3D	2.41	0.49
2:2:138:ASP:HA	16:2:610:CHL:O1D	2.11	0.49
3:3:181:GLU:OE1	3:3:184:ARG:NH1	2.45	0.49
4:4:264:PHE:CB	12:4:501:LUT:H24	2.42	0.49
5:A:440:HIS:O	5:A:444:VAL:HG23	2.12	0.49
6:B:205:GLY:HA3	6:B:247:THR:HA	1.94	0.49
6:B:438:TYR:HE1	6:B:519:LEU:HD13	1.77	0.49
1:1:81:TRP:CD1	15:1:612:CLA:HMD3	2.46	0.49
2:2:263:PHE:CE1	15:2:615:CLA:HAC2	2.47	0.49
4:4:203:GLN:O	4:4:207:ILE:HG13	2.11	0.49
15:4:605:CLA:HBA2	15:4:605:CLA:CBD	2.42	0.49
15:A:1139:CLA:H52	11:J:14:VAL:HG23	1.93	0.49
5:A:564:PRO:HG2	8:D:137:GLN:HA	1.93	0.49
15:B:1204:CLA:HED2	15:B:1204:CLA:H2A	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:83:ILE:HB	8:D:122:ILE:HG22	1.94	0.49
5:A:561:ARG:CZ	8:D:90:GLY:H	2.26	0.49
1:1:57:ASP:OD2	1:1:60:GLU:HA	2.12	0.49
16:1:610:CHL:HHD	16:1:610:CHL:HBC3	1.94	0.49
15:A:1013:CLA:HMA1	15:A:1013:CLA:C4	2.43	0.49
15:A:1119:CLA:HBA1	15:A:1123:CLA:HBB1	1.94	0.49
5:A:540:ALA:O	5:A:544:HIS:ND1	2.29	0.49
5:A:667:ALA:HB1	15:A:1106:CLA:HMC1	1.94	0.49
6:B:143:LEU:HD21	14:B:4003:BCR:H401	1.93	0.49
6:B:191:TRP:O	6:B:195:LEU:HD13	2.12	0.49
6:B:54:GLN:NE2	6:B:58:ILE:HD11	2.26	0.49
1:1:127:ILE:HD12	15:1:613:CLA:C2D	2.43	0.49
3:3:101:GLY:HA3	5:A:19:ARG:CD	2.35	0.49
3:3:205:LEU:HA	3:3:218:PRO:HD2	1.94	0.49
3:3:250:MET:CE	13:3:502:XAT:H10	2.42	0.49
16:4:611:CHL:HAA1	16:4:611:CHL:HBD	1.93	0.49
15:4:605:CLA:HED2	15:4:612:CLA:C1	2.43	0.49
15:A:1141:CLA:C1B	14:A:4004:BCR:H402	2.43	0.49
6:B:395:PHE:CE2	6:B:413:LEU:HD21	2.47	0.49
1:1:214:PHE:CE1	15:1:608:CLA:HMA1	2.47	0.49
2:2:208:MET:HE1	15:2:601:CLA:H43	1.93	0.49
15:2:604:CLA:HHD	16:2:609:CHL:HBB2	1.95	0.49
3:3:168:THR:O	3:3:172:ILE:HG12	2.12	0.49
3:3:176:ALA:O	14:3:503:BCR:H16C	2.12	0.49
5:A:558:ARG:HD3	5:A:567:ALA:HB2	1.94	0.49
6:B:434:THR:CG2	15:B:1021:CLA:H192	2.43	0.49
15:B:1223:CLA:HBB1	15:B:1223:CLA:HMB1	1.95	0.49
7:C:23:LEU:HD13	7:C:47:ASP:O	2.13	0.49
1:1:83:MET:CE	15:1:601:CLA:HAB	2.43	0.49
2:2:239:GLN:HE21	2:2:250:ASN:CB	2.26	0.49
25:A:2001:PQN:H141	14:B:4006:BCR:H333	1.95	0.49
2:2:145:LYS:HG2	4:4:333:PHE:CD1	2.48	0.49
2:2:113:ALA:CB	13:2:502:XAT:H402	2.42	0.49
16:2:609:CHL:HMB2	15:3:615:CLA:HED2	1.95	0.49
4:4:275:GLU:HG3	15:4:601:CLA:HMA1	1.93	0.49
4:4:325:VAL:HG13	4:4:328:PRO:CG	2.43	0.49
15:A:1104:CLA:H143	15:A:1127:CLA:HBB2	1.94	0.49
15:A:1134:CLA:CHA	15:A:1134:CLA:HBA1	2.41	0.49
5:A:398:GLY:O	5:A:402:VAL:HG23	2.12	0.49
6:B:288:ALA:HB2	15:B:1216:CLA:HBC2	1.95	0.49
6:B:128:ILE:HD12	15:B:1211:CLA:CMA	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:106:LEU:HD21	10:F:120:GLN:OE1	2.13	0.49
16:1:610:CHL:CBB	16:1:610:CHL:HHC	2.40	0.49
2:2:169:ARG:O	2:2:169:ARG:HD2	2.12	0.49
15:A:1132:CLA:HMB1	15:A:1132:CLA:HBB1	1.94	0.49
15:B:1201:CLA:HMB1	15:B:1201:CLA:CBB	2.43	0.49
15:B:1234:CLA:H12	15:B:1235:CLA:O1A	2.13	0.49
6:B:87:PRO:HB3	6:B:122:TYR:CE2	2.47	0.49
15:F:1301:CLA:HBC2	11:J:18:TRP:CH2	2.47	0.49
4:4:212:LEU:O	4:4:214:THR:N	2.46	0.49
5:A:492:PHE:O	5:A:495:PRO:HD2	2.12	0.49
15:B:1235:CLA:HBB1	15:B:1235:CLA:HMB1	1.95	0.49
6:B:441:ASN:O	6:B:445:GLN:HG2	2.12	0.49
6:B:53:GLY:O	6:B:57:ILE:HG12	2.12	0.49
10:F:125:ARG:O	10:F:129:ARG:HG3	2.13	0.49
1:1:171:GLU:HA	1:1:174:LYS:HD3	1.95	0.48
1:1:206:LEU:O	1:1:210:LEU:HD13	2.13	0.48
15:1:601:CLA:CMD	15:1:611:CLA:HBA2	2.42	0.48
2:2:184:PHE:CE1	2:2:185:LEU:HD13	2.46	0.48
14:3:504:BCR:H383	14:A:4002:BCR:H381	1.94	0.48
13:3:502:XAT:H183	15:3:606:CLA:CAB	2.43	0.48
15:A:1012:CLA:CBB	15:A:1012:CLA:HMB1	2.42	0.48
5:A:221:SER:HA	5:A:291:LEU:HD12	1.94	0.48
5:A:446:ILE:HA	15:B:1023:CLA:O1A	2.13	0.48
8:D:181:GLY:C	8:D:182:ARG:HD2	2.32	0.48
1:1:85:GLY:HA2	13:1:502:XAT:H382	1.95	0.48
14:3:503:BCR:C21	15:3:613:CLA:HBA1	2.44	0.48
4:4:172:TRP:HE1	13:4:502:XAT:C19	2.26	0.48
5:A:190:TRP:CH2	15:A:1108:CLA:HMB3	2.48	0.48
5:A:297:HIS:O	5:A:301:ILE:HG12	2.13	0.48
5:A:301:ILE:HG23	5:A:305:PHE:CD2	2.47	0.48
5:A:57:HIS:ND1	15:A:1104:CLA:HBA1	2.27	0.48
5:A:96:ALA:HB2	5:A:159:LEU:CB	2.42	0.48
6:B:175:ARG:HE	15:B:1221:CLA:HMD1	1.78	0.48
10:F:120:GLN:O	10:F:124:GLU:HG3	2.13	0.48
15:F:1302:CLA:HMC3	14:F:4002:BCR:H331	1.94	0.48
11:J:8:LEU:CA	11:J:13:VAL:HG11	2.43	0.48
3:3:133:LEU:HD11	3:3:138:VAL:HG21	1.94	0.48
3:3:170:PHE:CD1	15:3:610:CLA:HBD	2.49	0.48
5:A:415:ARG:HH12	15:A:1128:CLA:HED3	1.78	0.48
2:2:137:TYR:O	2:2:138:ASP:OD1	2.32	0.48
15:3:611:CLA:HBA2	15:3:611:CLA:C4A	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:605:CLA:C1	10:F:219:LEU:HG	2.44	0.48
5:A:299:LEU:HD21	15:A:1113:CLA:CMC	2.42	0.48
5:A:443:TRP:CE3	15:A:1130:CLA:HAB	2.48	0.48
5:A:382:THR:HB	5:A:520:LYS:HZ2	1.77	0.48
15:B:1211:CLA:HMA1	14:B:4003:BCR:H271	1.96	0.48
5:A:702:TRP:CZ3	6:B:418:ALA:HB2	2.49	0.48
7:C:60:THR:HG22	7:C:62:PHE:O	2.13	0.48
15:A:1126:CLA:O1D	15:A:1127:CLA:HMA1	2.13	0.48
5:A:521:VAL:HG11	5:A:627:VAL:HG21	1.95	0.48
6:B:69:VAL:HG21	6:B:125:TRP:CZ3	2.48	0.48
6:B:182:GLY:HA3	15:B:1210:CLA:CBB	2.43	0.48
6:B:191:TRP:CE2	6:B:195:LEU:HD11	2.48	0.48
8:D:174:TYR:HB3	8:D:176:GLU:CD	2.33	0.48
11:J:37:LEU:O	11:J:37:LEU:HG	2.13	0.48
15:J:1302:CLA:C2C	14:J:4002:BCR:H10C	2.43	0.48
1:1:221:ASN:HD21	15:1:603:CLA:CAD	2.26	0.48
1:1:85:GLY:HA2	13:1:502:XAT:C38	2.44	0.48
2:2:115:LEU:HD11	15:2:601:CLA:CBC	2.43	0.48
5:A:77:HIS:CB	15:A:1111:CLA:HED2	2.42	0.48
15:B:1203:CLA:CBB	15:B:1203:CLA:HMB1	2.44	0.48
15:B:1235:CLA:CBB	15:B:1235:CLA:HMB1	2.43	0.48
6:B:24:TYR:CD1	21:B:5002:DGD:HG32	2.48	0.48
11:J:27:ILE:CG2	14:J:4002:BCR:H343	2.43	0.48
1:1:166:ASP:HB3	1:1:169:SER:OG	2.14	0.48
1:1:170:PHE:O	1:1:174:LYS:HG3	2.14	0.48
1:1:44:LYS:HB3	1:1:46:TYR:CE2	2.49	0.48
1:1:46:TYR:OH	1:1:60:GLU:HG3	2.12	0.48
15:4:604:CLA:H43	10:F:219:LEU:CD2	2.43	0.48
5:A:395:MET:HE3	5:A:606:VAL:HG11	1.95	0.48
15:B:1218:CLA:HAB	15:B:1219:CLA:H2	1.95	0.48
6:B:381:GLY:HA3	6:B:584:MET:CE	2.41	0.48
6:B:69:VAL:HG13	6:B:122:TYR:CE1	2.41	0.48
10:F:115:PRO:O	10:F:119:LEU:HD13	2.14	0.48
15:1:606:CLA:HBA2	15:1:606:CLA:CHA	2.39	0.48
4:4:178:VAL:HG21	12:4:501:LUT:H401	1.95	0.48
15:A:1106:CLA:C1C	15:A:1107:CLA:HMD2	2.44	0.48
5:A:153:ILE:HD13	5:A:159:LEU:HD21	1.96	0.48
5:A:297:HIS:HB2	15:A:1116:CLA:HMA3	1.95	0.48
5:A:81:LEU:HD12	15:A:1111:CLA:CED	2.43	0.48
6:B:168:TRP:CZ2	15:B:1210:CLA:HAC2	2.48	0.48
1:1:64:GLU:HG2	1:1:66:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:222:GLU:HB3	15:2:601:CLA:HMB3	1.95	0.48
13:2:502:XAT:H31	13:2:502:XAT:H391	1.75	0.48
2:2:199:PRO:HD2	15:2:601:CLA:CED	2.44	0.48
5:A:403:VAL:HG11	5:A:596:LEU:CD2	2.44	0.48
5:A:408:HIS:HA	5:A:411:ILE:HD12	1.95	0.48
5:A:451:HIS:HA	15:A:1132:CLA:HBB2	1.96	0.48
5:A:677:PHE:CG	14:A:4006:BCR:H363	2.48	0.48
5:A:690:ARG:NH1	6:B:567:GLY:O	2.46	0.48
15:B:1210:CLA:HMB1	15:B:1210:CLA:CBB	2.44	0.48
6:B:440:HIS:O	6:B:444:VAL:HG23	2.14	0.48
6:B:92:ILE:HG22	6:B:94:ASP:H	1.77	0.48
8:D:157:ARG:HH21	8:D:165:GLN:HB3	1.79	0.48
10:F:173:TYR:HA	10:F:217:TRP:HZ2	1.77	0.48
1:1:134:ALA:HB1	14:1:503:BCR:H363	1.96	0.48
2:2:261:VAL:HG22	2:2:262:THR:H	1.79	0.48
15:A:1138:CLA:HMC3	15:A:1139:CLA:C4D	2.44	0.48
5:A:44:ASN:OD1	9:E:109:GLN:HG3	2.14	0.48
5:A:638:SER:O	5:A:644:GLY:HA3	2.14	0.48
6:B:214:LEU:HD23	6:B:214:LEU:H	1.78	0.48
6:B:346:THR:HB	6:B:380:ALA:HB2	1.94	0.48
6:B:74:ASN:HB2	6:B:77:GLN:HB2	1.96	0.48
1:1:218:PHE:HA	1:1:221:ASN:HD21	1.79	0.47
15:A:1116:CLA:H43	15:A:1133:CLA:HAA2	1.96	0.47
15:A:1126:CLA:C1C	14:A:4006:BCR:HC22	2.44	0.47
5:A:687:PHE:HB2	15:A:1013:CLA:HBC2	1.93	0.47
15:B:1231:CLA:HMB1	15:B:1231:CLA:HBB1	1.96	0.47
6:B:358:PRO:HG3	15:B:1215:CLA:CAA	2.43	0.47
6:B:124:TRP:HB2	6:B:359:TYR:CE2	2.49	0.47
6:B:441:ASN:ND2	6:B:615:THR:O	2.47	0.47
9:E:78:ARG:HE	9:E:123:GLU:CD	2.17	0.47
14:B:4006:BCR:C21	15:F:1301:CLA:HAB	2.44	0.47
14:J:4002:BCR:H23C	14:J:4002:BCR:H392	1.96	0.47
4:4:174:MET:HB3	12:4:501:LUT:C34	2.45	0.47
24:A:1011:CL0:H13	15:A:1012:CLA:CAD	2.44	0.47
5:A:118:VAL:HG13	5:A:138:ILE:HD11	1.96	0.47
6:B:316:LEU:HD22	6:B:408:VAL:HG12	1.96	0.47
6:B:408:VAL:O	6:B:412:VAL:HG23	2.13	0.47
6:B:423:LEU:HB3	6:B:533:LEU:HD13	1.95	0.47
6:B:435:LEU:O	6:B:439:VAL:HG23	2.14	0.47
11:J:9:SER:HA	11:J:13:VAL:CG2	2.41	0.47
15:A:1012:CLA:HMB3	15:B:1021:CLA:C19	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:190:TRP:HH2	15:A:1108:CLA:HMB3	1.79	0.47
5:A:464:ALA:HB3	15:B:1206:CLA:HMC1	1.94	0.47
5:A:667:ALA:HB3	15:A:1106:CLA:CBC	2.44	0.47
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.65	0.47
7:C:10:THR:HA	9:E:100:TYR:HE2	1.79	0.47
11:J:13:VAL:O	11:J:14:VAL:C	2.53	0.47
12:1:501:LUT:H31	12:1:501:LUT:H391	1.54	0.47
13:1:502:XAT:H403	15:1:605:CLA:HMC2	1.95	0.47
15:1:608:CLA:HBB1	15:1:608:CLA:HHC	1.96	0.47
2:2:270:ILE:N	2:2:271:PRO:HD3	2.29	0.47
3:3:104:VAL:O	3:3:104:VAL:HG23	2.15	0.47
3:3:85:ASP:OD2	16:3:604:CHL:HBA1	2.14	0.47
5:A:223:PRO:HG3	5:A:243:PHE:HE2	1.80	0.47
5:A:593:PHE:CE1	5:A:728:VAL:HB	2.49	0.47
6:B:125:TRP:HB3	6:B:130:LEU:HD12	1.96	0.47
6:B:189:LEU:O	6:B:192:THR:OG1	2.24	0.47
6:B:347:SER:O	6:B:351:GLN:HG2	2.14	0.47
15:A:1012:CLA:CMA	6:B:617:LEU:HD13	2.38	0.47
7:C:24:ASP:OD1	8:D:175:PRO:HG2	2.15	0.47
1:1:206:LEU:HD23	1:1:210:LEU:HD13	1.96	0.47
15:2:606:CLA:CBB	15:2:606:CLA:HMB1	2.44	0.47
15:2:605:CLA:CAC	15:2:612:CLA:HAA1	2.31	0.47
4:4:311:HIS:HA	4:4:318:VAL:CG2	2.45	0.47
4:4:318:VAL:HB	15:4:603:CLA:HED1	1.95	0.47
4:4:178:VAL:CG2	12:4:501:LUT:H401	2.45	0.47
15:4:602:CLA:CBB	15:4:602:CLA:HMB1	2.44	0.47
4:4:258:GLY:HA2	16:4:611:CHL:CMD	2.45	0.47
21:4:811:DGD:HA51	15:B:1230:CLA:H12	1.97	0.47
5:A:105:LEU:HD12	5:A:149:ARG:HH11	1.79	0.47
14:A:4002:BCR:C6	14:A:4002:BCR:H342	2.45	0.47
5:A:97:ARG:HA	5:A:160:TYR:OH	2.13	0.47
15:B:1218:CLA:HMB1	15:B:1218:CLA:HBB1	1.96	0.47
15:B:1221:CLA:CBB	15:B:1221:CLA:HMB1	2.44	0.47
15:B:1225:CLA:ND	14:B:4002:BCR:H282	2.30	0.47
7:C:63:LEU:O	8:D:192:ILE:HD13	2.14	0.47
10:F:166:ILE:HD12	10:F:167:PRO:N	2.29	0.47
1:1:183:LEU:CD1	15:1:607:CLA:HMD3	2.44	0.47
16:1:610:CHL:OMC	16:1:610:CHL:HAC2	2.13	0.47
12:3:501:LUT:H222	15:3:601:CLA:C4	2.45	0.47
3:3:281:ILE:N	15:3:603:CLA:HED1	2.30	0.47
15:A:1122:CLA:CBC	14:A:4004:BCR:HC8	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:266:THR:HG21	6:B:360:ALA:HB1	1.95	0.47
6:B:173:GLU:HB3	6:B:292:TYR:HB3	1.97	0.47
8:D:152:THR:HA	8:D:174:TYR:OH	2.15	0.47
6:B:452:LYS:HD2	10:F:129:ARG:NE	2.30	0.47
10:F:126:THR:OG1	10:F:129:ARG:NH1	2.48	0.47
15:A:1132:CLA:HMB1	15:A:1132:CLA:CBB	2.45	0.47
5:A:700:ILE:HD13	15:A:1138:CLA:HMD1	1.96	0.47
6:B:188:SER:HB3	6:B:282:ALA:HB2	1.96	0.47
10:F:224:GLU:OE2	10:F:230:LEU:HB3	2.14	0.47
2:2:74:PRO:HB3	2:2:76:TRP:CZ2	2.50	0.47
4:4:218:ILE:CD1	16:4:613:CHL:HED2	2.44	0.47
5:A:367:VAL:HG11	15:A:1127:CLA:HMD3	1.97	0.47
5:A:344:ILE:HD13	5:A:422:ASN:HB3	1.95	0.47
5:A:448:LEU:HB2	5:A:541:PHE:HD1	1.79	0.47
6:B:57:ILE:HG13	15:B:1201:CLA:HBB1	1.95	0.47
7:C:61:ASP:HA	7:C:62:PHE:HA	1.66	0.47
2:2:254:HIS:CD2	15:2:603:CLA:HAA2	2.49	0.47
2:2:168:LYS:HE3	16:2:611:CHL:OMC	2.14	0.47
2:2:65:PRO:HG2	17:2:801:LHG:O2	2.14	0.47
3:3:131:GLU:OE1	3:3:264:PRO:HD2	2.14	0.47
15:2:607:CLA:CAB	14:3:503:BCR:HC31	2.45	0.47
3:3:81:ASP:HA	16:3:604:CHL:HED2	1.96	0.47
25:A:2001:PQN:H161	25:A:2001:PQN:H141	1.43	0.47
5:A:306:LEU:O	5:A:310:HIS:ND1	2.44	0.47
5:A:68:GLU:HB2	5:A:71:ARG:HH21	1.80	0.47
6:B:718:TYR:HE1	15:B:1021:CLA:O2A	1.97	0.47
15:B:1223:CLA:HMB1	15:B:1223:CLA:CBB	2.45	0.47
11:J:21:PHE:CE1	14:J:4003:BCR:HC21	2.50	0.47
14:1:503:BCR:H24C	15:1:613:CLA:O2A	2.15	0.47
2:2:198:TYR:HD2	2:2:215:PHE:CZ	2.32	0.47
2:2:230:MET:SD	15:2:604:CLA:HMC3	2.55	0.47
13:3:502:XAT:H21	15:3:613:CLA:HMC2	1.97	0.47
15:A:1103:CLA:H72	15:A:1111:CLA:O2A	2.15	0.47
5:A:57:HIS:HB2	15:A:1128:CLA:O1A	2.15	0.47
6:B:198:VAL:C	6:B:201:PRO:HD2	2.35	0.47
10:F:106:LEU:HD13	10:F:119:LEU:CB	2.45	0.47
1:1:182:ARG:HH22	15:1:604:CLA:HED2	1.79	0.47
15:1:604:CLA:HBC2	16:1:609:CHL:HBB2	1.96	0.47
1:1:215:PHE:CD1	4:4:212:LEU:HD22	2.50	0.47
12:4:501:LUT:H32	15:4:601:CLA:CAB	2.45	0.47
15:A:1112:CLA:HHB	14:A:4002:BCR:H331	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1124:CLA:HBB2	14:A:4005:BCR:H392	1.96	0.47
6:B:411:ARG:HD3	15:B:1227:CLA:OBD	2.15	0.47
15:B:1228:CLA:H102	15:B:1229:CLA:H162	1.95	0.47
6:B:494:TRP:HE1	15:B:1231:CLA:HED2	1.80	0.47
10:F:166:ILE:N	10:F:167:PRO:CD	2.78	0.47
15:B:1235:CLA:H41	14:F:4002:BCR:H321	1.96	0.47
13:3:502:XAT:H192	15:3:606:CLA:CBB	2.43	0.46
5:A:484:ALA:HB2	15:A:1136:CLA:HED2	1.97	0.46
6:B:243:HIS:ND1	6:B:251:SER:HA	2.30	0.46
6:B:244:ALA:HB2	6:B:249:ASP:HB2	1.97	0.46
6:B:85:VAL:HG22	6:B:86:ARG:N	2.30	0.46
8:D:75:LEU:HD13	8:D:102:VAL:HG11	1.96	0.46
9:E:117:ASN:OD1	9:E:118:ASN:N	2.48	0.46
9:E:77:LEU:HB2	9:E:123:GLU:O	2.16	0.46
14:1:503:BCR:H393	15:1:606:CLA:C1C	2.45	0.46
2:2:270:ILE:O	2:2:270:ILE:HG22	2.15	0.46
4:4:222:LEU:HG	14:4:503:BCR:C16	2.46	0.46
14:A:4004:BCR:H351	14:A:4004:BCR:H15C	1.64	0.46
5:A:546:THR:OG1	5:A:598:TRP:HB3	2.16	0.46
5:A:54:ALA:HB2	17:A:5002:LHG:O9	2.15	0.46
5:A:615:GLN:OE1	5:A:653:GLN:NE2	2.48	0.46
5:A:672:PHE:HE2	6:B:621:LEU:HD21	1.80	0.46
6:B:478:LEU:CD1	15:B:1232:CLA:HMC3	2.44	0.46
6:B:131:ARG:HH11	6:B:207:HIS:CE1	2.33	0.46
5:A:119:TRP:CZ2	14:J:4002:BCR:H332	2.50	0.46
4:4:318:VAL:HG23	4:4:318:VAL:O	2.15	0.46
2:2:168:LYS:HG2	15:4:609:CLA:CED	2.45	0.46
15:A:1129:CLA:CBB	15:A:1129:CLA:HMB1	2.45	0.46
3:3:101:GLY:CA	5:A:19:ARG:HD2	2.34	0.46
5:A:659:GLN:O	5:A:659:GLN:HG2	2.16	0.46
7:C:29:VAL:HA	8:D:178:VAL:HG13	1.98	0.46
11:J:12:PRO:HB3	14:J:4002:BCR:H291	1.97	0.46
10:F:201:ILE:HG23	11:J:9:SER:HB2	1.96	0.46
3:3:121:MET:HG3	3:3:243:GLY:HA2	1.96	0.46
3:3:206:PHE:HD1	3:3:220:PHE:HE2	1.63	0.46
3:3:248:LEU:HG	16:3:604:CHL:HAC1	1.97	0.46
5:A:57:HIS:NE2	15:A:1103:CLA:HBB2	2.30	0.46
5:A:392:THR:HG22	15:A:1126:CLA:CAB	2.45	0.46
5:A:119:TRP:CG	14:J:4002:BCR:HC41	2.50	0.46
5:A:190:TRP:HA	5:A:193:ASN:OD1	2.15	0.46
6:B:346:THR:OG1	15:B:1225:CLA:HAC1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1235:CLA:H142	15:B:1235:CLA:H111	1.69	0.46
1:1:71:TYR:OH	15:B:1240:CLA:HAB	2.16	0.46
6:B:468:GLN:HE21	6:B:510:PHE:HE2	1.62	0.46
6:B:631:GLN:HE22	6:B:733:ARG:HE	1.62	0.46
10:F:103:ASP:HA	10:F:106:LEU:HB3	1.96	0.46
10:F:217:TRP:CD1	10:F:218:PRO:HD3	2.50	0.46
15:1:608:CLA:HHC	15:1:608:CLA:CBB	2.46	0.46
2:2:155:ILE:HG12	16:2:610:CHL:HBC3	1.97	0.46
16:2:609:CHL:HED1	3:3:182:LEU:HB3	1.97	0.46
5:A:700:ILE:HD13	15:A:1138:CLA:CMD	2.46	0.46
5:A:612:TRP:HB2	5:A:649:PHE:CD1	2.49	0.46
6:B:283:VAL:HG21	15:B:1213:CLA:HAB	1.97	0.46
6:B:349:VAL:O	6:B:353:MET:HG3	2.16	0.46
6:B:460:PHE:HB3	15:B:1234:CLA:H2	1.97	0.46
10:F:113:SER:OG	10:F:115:PRO:HD2	2.16	0.46
1:1:83:MET:HE2	15:1:601:CLA:HAB	1.97	0.46
2:2:235:GLY:O	2:2:239:GLN:HB3	2.15	0.46
4:4:285:LEU:HD21	15:4:602:CLA:CAC	2.45	0.46
15:A:1103:CLA:CMC	15:A:1128:CLA:HMA1	2.41	0.46
6:B:198:VAL:HG11	15:B:1211:CLA:O1D	2.15	0.46
6:B:438:TYR:CD2	6:B:617:LEU:HD21	2.51	0.46
12:1:501:LUT:C24	12:1:501:LUT:H363	2.46	0.46
13:1:502:XAT:H12	15:1:605:CLA:CMB	2.45	0.46
2:2:236:PHE:CE1	12:2:501:LUT:H363	2.39	0.46
3:3:135:LYS:HE2	3:3:135:LYS:HA	1.98	0.46
4:4:289:ALA:HB2	12:4:501:LUT:C9	2.46	0.46
15:A:1110:CLA:CGA	15:A:1110:CLA:C1A	2.94	0.46
5:A:443:TRP:CZ2	15:A:1131:CLA:HMD1	2.51	0.46
5:A:180:HIS:O	5:A:185:ALA:HA	2.15	0.46
5:A:345:LEU:CB	15:A:1123:CLA:HBC3	2.44	0.46
5:A:737:ALA:HA	14:A:4006:BCR:HC42	1.98	0.46
5:A:372:TYR:CD2	5:A:610:PHE:HE1	2.34	0.46
15:B:1228:CLA:H52	14:F:4002:BCR:H372	1.97	0.46
15:B:1231:CLA:H62	15:B:1231:CLA:H92	1.82	0.46
6:B:416:LYS:O	6:B:420:ILE:HG12	2.15	0.46
6:B:370:ALA:HA	6:B:595:TRP:CZ3	2.51	0.46
11:J:11:ALA:O	11:J:16:LEU:HD23	2.16	0.46
1:1:128:LEU:O	1:1:132:VAL:HG23	2.15	0.46
15:1:603:CLA:HMB1	15:1:603:CLA:HBB1	1.98	0.46
1:1:154:PRO:CG	15:1:611:CLA:HMD2	2.42	0.46
2:2:198:TYR:CE2	2:2:219:LYS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:272:HIS:HB2	15:A:1114:CLA:OBD	2.16	0.46
2:2:113:ALA:CA	13:2:502:XAT:H402	2.46	0.46
5:A:246:ASN:ND2	5:A:249:ILE:HG12	2.30	0.46
5:A:494:ALA:HA	5:A:498:THR:OG1	2.16	0.46
15:B:1232:CLA:CBB	15:B:1232:CLA:HMB1	2.46	0.46
6:B:22:ILE:HD11	6:B:696:ASP:OD2	2.16	0.46
6:B:339:LEU:O	6:B:383:ILE:HG22	2.16	0.46
6:B:460:PHE:HB2	15:B:1235:CLA:CAD	2.46	0.46
7:C:22:PRO:HB3	7:C:53:ARG:NH1	2.31	0.46
14:1:503:BCR:H271	15:1:606:CLA:NC	2.31	0.46
1:1:46:TYR:CD1	1:1:63:LYS:HG3	2.50	0.46
15:A:1013:CLA:C3	15:A:1013:CLA:HMA1	2.45	0.46
15:A:1121:CLA:HHC	15:A:1121:CLA:CBB	2.46	0.46
5:A:647:ARG:NH2	6:B:636:TYR:O	2.49	0.46
5:A:668:TYR:HE1	15:A:1106:CLA:HAC1	1.81	0.46
5:A:682:SER:HB2	5:A:727:GLY:O	2.16	0.46
24:A:1011:CL0:H16	15:B:1021:CLA:HAA1	1.96	0.46
7:C:33:GLY:H	7:C:37:ALA:CB	2.29	0.46
7:C:52:LYS:HE2	7:C:69:LEU:HD21	1.98	0.46
2:2:114:MET:HB3	12:2:501:LUT:C14	2.46	0.46
15:A:1012:CLA:HMB3	15:B:1021:CLA:C20	2.44	0.46
5:A:199:ASN:O	5:A:203:ALA:HB3	2.16	0.46
5:A:43:PRO:HB3	5:A:48:TRP:CD2	2.50	0.46
5:A:675:ALA:HA	5:A:678:VAL:HG22	1.98	0.46
15:B:1218:CLA:CBB	15:B:1218:CLA:HMB1	2.46	0.46
15:B:1219:CLA:CBB	15:B:1219:CLA:HMB1	2.46	0.46
5:A:580:ARG:HA	7:C:77:LEU:HA	1.97	0.46
1:1:69:GLN:OE1	1:1:152:LEU:HD11	2.16	0.45
16:1:610:CHL:CGA	16:1:610:CHL:HBD	2.46	0.45
15:A:1136:CLA:CMA	15:A:1137:CLA:HED2	2.45	0.45
5:A:344:ILE:HG23	5:A:412:PHE:CZ	2.51	0.45
5:A:46:THR:CG2	5:A:715:PRO:HA	2.46	0.45
15:B:1231:CLA:HMB1	15:B:1231:CLA:CBB	2.46	0.45
6:B:715:SER:O	6:B:719:ILE:HG12	2.16	0.45
5:A:580:ARG:NH1	7:C:51:CYS:HB3	2.29	0.45
5:A:300:ALA:HA	15:A:1115:CLA:HMC3	1.98	0.45
5:A:179:PHE:O	5:A:184:ALA:N	2.49	0.45
5:A:21:PRO:HG3	5:A:185:ALA:CB	2.46	0.45
5:A:21:PRO:HG3	5:A:185:ALA:HB3	1.97	0.45
15:A:1012:CLA:HMB3	15:B:1021:CLA:C18	2.46	0.45
15:B:1220:CLA:H93	15:B:1220:CLA:H61	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1012:CLA:C4	6:B:439:VAL:HG13	2.46	0.45
6:B:69:VAL:HG21	6:B:125:TRP:HZ3	1.81	0.45
16:2:609:CHL:HBC3	17:2:801:LHG:HC42	1.98	0.45
2:2:93:SER:HB2	2:2:99:ARG:HA	1.97	0.45
3:3:253:TYR:OH	12:3:501:LUT:H8	2.16	0.45
3:3:121:MET:HE1	15:3:601:CLA:HMC3	1.98	0.45
4:4:263:ILE:CG2	16:4:611:CHL:H11	2.46	0.45
5:A:396:TRP:HB3	15:A:1126:CLA:HMC3	1.97	0.45
5:A:13:VAL:HG11	5:A:196:SER:HB2	1.98	0.45
5:A:233:ASP:OD1	5:A:234:PRO:HD2	2.15	0.45
5:A:351:ALA:HB2	5:A:412:PHE:CE1	2.51	0.45
5:A:32:PRO:HB2	5:A:48:TRP:CH2	2.50	0.45
5:A:417:TYR:HD2	5:A:558:ARG:HH21	1.64	0.45
5:A:721:THR:HB	17:A:5002:LHG:HC41	1.97	0.45
15:B:1214:CLA:H41	15:B:1232:CLA:HMA2	1.98	0.45
6:B:327:VAL:HG13	6:B:333:PHE:HD2	1.82	0.45
1:1:72:ARG:O	1:1:76:LEU:HD13	2.17	0.45
18:1:802:LMG:HC2	18:1:802:LMG:HC71	1.55	0.45
2:2:141:LYS:O	2:2:145:LYS:HG3	2.16	0.45
15:2:604:CLA:HMD2	16:2:609:CHL:CBB	2.46	0.45
2:2:78:ASP:OD1	2:2:79:GLY:N	2.48	0.45
3:3:199:PHE:HZ	14:3:503:BCR:H10C	1.79	0.45
14:3:504:BCR:HC31	15:3:615:CLA:HMC3	1.97	0.45
5:A:121:ILE:HG23	5:A:122:VAL:H	1.81	0.45
5:A:721:THR:CG2	17:A:5002:LHG:HC41	2.46	0.45
5:A:50:TRP:HE1	15:A:1139:CLA:CBB	2.29	0.45
15:B:1217:CLA:CBB	15:B:1217:CLA:HHC	2.46	0.45
15:B:1221:CLA:C2	15:B:1221:CLA:HMA2	2.46	0.45
5:A:584:CYS:N	6:B:670:GLY:HA3	2.14	0.45
4:4:124:ARG:HB2	4:4:145:TYR:CE1	2.51	0.45
4:4:314:ASP:O	4:4:318:VAL:HG22	2.17	0.45
4:4:325:VAL:HG13	4:4:328:PRO:CD	2.46	0.45
15:A:1105:CLA:HMB3	15:A:1106:CLA:CMA	2.46	0.45
15:A:1132:CLA:HMD3	15:B:1206:CLA:CAB	2.46	0.45
5:A:382:THR:HB	5:A:520:LYS:NZ	2.31	0.45
5:A:618:VAL:HG12	5:A:619:TRP:CD1	2.52	0.45
6:B:349:VAL:HG11	15:B:1225:CLA:HMD3	1.97	0.45
7:C:4:VAL:CG2	8:D:207:SER:HB2	2.45	0.45
10:F:79:ILE:HD11	10:F:158:PHE:CZ	2.51	0.45
11:J:11:ALA:N	11:J:12:PRO:HD2	2.31	0.45
24:A:1011:CL0:H10	24:A:1011:CL0:H72	1.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1102:CLA:HED2	15:A:1102:CLA:H2A	1.99	0.45
15:A:1140:CLA:H41	15:A:1140:CLA:H61	1.47	0.45
5:A:494:ALA:O	5:A:499:ALA:N	2.49	0.45
5:A:564:PRO:HG3	8:D:137:GLN:HG2	1.98	0.45
15:B:1023:CLA:H3A	15:B:1023:CLA:CGA	2.46	0.45
5:A:706:LYS:HE2	15:B:1228:CLA:HED1	1.98	0.45
6:B:306:LEU:O	6:B:320:HIS:HB2	2.17	0.45
6:B:87:PRO:HB2	6:B:117:ALA:HB3	1.98	0.45
10:F:83:THR:CG2	10:F:84:PRO:HD2	2.47	0.45
16:2:609:CHL:HBD	16:2:609:CHL:HAA2	1.99	0.45
3:3:246:ALA:HB2	12:3:501:LUT:C20	2.40	0.45
15:3:605:CLA:HAC1	15:3:612:CLA:HBC2	1.98	0.45
12:4:501:LUT:H15	12:4:501:LUT:H201	1.79	0.45
5:A:197:MET:HB3	15:A:1123:CLA:HMD1	1.98	0.45
5:A:283:ASN:OD1	5:A:284:PRO:HD2	2.17	0.45
15:B:1021:CLA:H3A	15:B:1021:CLA:HBA1	1.30	0.45
6:B:105:PHE:O	6:B:113:PRO:HA	2.17	0.45
15:B:1237:CLA:HMB1	15:B:1237:CLA:CBB	2.47	0.45
6:B:54:GLN:HB2	15:B:1202:CLA:HMB2	1.99	0.45
9:E:74:VAL:HG21	9:E:124:ILE:HG21	1.98	0.45
11:J:18:TRP:O	11:J:19:ALA:HB3	2.17	0.45
15:1:605:CLA:H2A	15:1:605:CLA:O1D	2.17	0.45
4:4:176:ALA:HA	15:4:606:CLA:CAB	2.43	0.45
5:A:57:HIS:CD2	15:A:1103:CLA:HBB2	2.51	0.45
5:A:256:SER:OG	5:A:274:ASP:HB2	2.17	0.45
5:A:443:TRP:CE2	15:A:1130:CLA:HAB	2.52	0.45
5:A:654:SER:O	5:A:658:ILE:HG12	2.17	0.45
6:B:658:TYR:CZ	15:B:1021:CLA:HMA2	2.52	0.45
6:B:510:PHE:CE1	15:B:1223:CLA:HBC2	2.52	0.45
6:B:498:TRP:CD1	15:B:1231:CLA:HED3	2.51	0.45
9:E:93:VAL:HG22	9:E:102:VAL:HG22	1.99	0.45
3:3:139:ILE:HG12	3:3:140:PRO:HD2	1.98	0.45
4:4:296:THR:C	4:4:298:ALA:H	2.20	0.45
24:A:1011:CL0:CBC	6:B:626:TRP:HB2	2.47	0.45
5:A:217:GLN:NE2	15:A:1117:CLA:O1D	2.50	0.45
13:2:502:XAT:C13	15:2:605:CLA:HMA3	2.47	0.45
13:3:502:XAT:H42	15:3:606:CLA:C1B	2.47	0.45
4:4:331:THR:HG23	4:4:331:THR:O	2.16	0.45
5:A:93:PHE:HE2	15:A:1105:CLA:HMD3	1.81	0.45
5:A:681:PHE:O	5:A:684:MET:HB3	2.16	0.45
15:B:1214:CLA:HBA2	15:B:1223:CLA:HBB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:2002:PQN:H261	25:B:2002:PQN:H222	1.62	0.45
8:D:208:GLU:HB2	8:D:210:PHE:CE1	2.52	0.45
10:F:186:ILE:HG13	10:F:190:LYS:NZ	2.31	0.45
1:1:77:ILE:HG23	15:1:611:CLA:HED3	1.99	0.44
2:2:233:PHE:CZ	13:2:502:XAT:H30	2.52	0.44
3:3:117:ALA:HB1	3:3:243:GLY:CA	2.36	0.44
3:3:200:LEU:O	3:3:200:LEU:HG	2.17	0.44
3:3:202:LEU:HD22	3:3:205:LEU:HD12	1.99	0.44
4:4:325:VAL:HG13	4:4:328:PRO:HD2	1.98	0.44
4:4:172:TRP:CH2	14:4:503:BCR:H371	2.50	0.44
5:A:684:MET:HB2	15:A:1013:CLA:CHC	2.47	0.44
6:B:175:ARG:HB2	15:B:1210:CLA:HBC3	1.99	0.44
9:E:91:VAL:CG2	9:E:105:ARG:HB2	2.47	0.44
10:F:101:VAL:O	10:F:104:LYS:HG2	2.16	0.44
15:A:1106:CLA:CAB	14:J:4001:BCR:H363	2.47	0.44
14:2:503:BCR:H271	15:2:606:CLA:NB	2.32	0.44
4:4:216:ALA:O	4:4:219:GLU:HB3	2.16	0.44
14:A:4005:BCR:C35	14:A:4005:BCR:C11	2.96	0.44
6:B:663:MET:HA	15:B:1023:CLA:C2C	2.47	0.44
6:B:219:HIS:ND1	6:B:220:PRO:O	2.49	0.44
6:B:277:HIS:O	6:B:281:ILE:HG12	2.17	0.44
6:B:438:TYR:HB3	6:B:617:LEU:HG	1.98	0.44
15:B:1240:CLA:HBA1	17:B:5001:LHG:HC41	1.99	0.44
8:D:128:ASN:OD1	8:D:129:LEU:N	2.51	0.44
8:D:132:PHE:HB3	8:D:137:GLN:OE1	2.17	0.44
8:D:157:ARG:NE	8:D:167:LEU:HB2	2.31	0.44
3:3:121:MET:CE	15:3:601:CLA:HMC3	2.47	0.44
14:3:503:BCR:C15	15:3:611:CLA:HMB3	2.47	0.44
15:3:606:CLA:HHD	15:3:606:CLA:HBC2	1.99	0.44
5:A:704:HIS:CE1	15:A:1139:CLA:HAC1	2.52	0.44
6:B:593:PHE:HE2	15:B:1021:CLA:H61	1.82	0.44
15:B:1219:CLA:HBC2	15:B:1220:CLA:CGA	2.48	0.44
6:B:646:VAL:O	6:B:650:THR:HG23	2.18	0.44
1:1:33:ARG:HH11	1:1:55:ASN:HB2	1.82	0.44
15:3:608:CLA:CBB	15:3:608:CLA:HHC	2.47	0.44
5:A:75:SER:HG	5:A:181:TYR:HB2	1.81	0.44
5:A:282:LEU:HB3	5:A:289:LEU:HD23	1.99	0.44
5:A:282:LEU:HD11	5:A:515:VAL:HG11	1.98	0.44
5:A:604:SER:HA	5:A:607:ILE:HG12	1.98	0.44
6:B:292:TYR:CE1	6:B:302:LEU:HD21	2.53	0.44
15:1:605:CLA:HMD2	15:1:612:CLA:ND	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:MET:O	12:1:501:LUT:H15	2.17	0.44
2:2:235:GLY:O	2:2:239:GLN:CB	2.66	0.44
3:3:145:VAL:HG22	3:3:146:ASP:N	2.33	0.44
23:B:5031:GSH:HN2	23:B:5031:GSH:C1	2.30	0.44
5:A:695:GLU:HB3	6:B:537:LYS:NZ	2.32	0.44
10:F:82:LEU:HB3	10:F:139:LEU:HB3	1.99	0.44
10:F:79:ILE:HG21	10:F:154:LEU:HD12	2.00	0.44
14:2:503:BCR:H321	14:2:503:BCR:C8	2.48	0.44
15:2:612:CLA:H12	18:2:802:LMG:HC72	2.00	0.44
12:3:501:LUT:H401	12:3:501:LUT:H35	1.78	0.44
24:A:1011:CL0:CGD	24:A:1011:CL0:H8	2.47	0.44
15:A:1135:CLA:CBB	15:A:1135:CLA:HMB1	2.48	0.44
5:A:392:THR:HG22	5:A:396:TRP:CD1	2.52	0.44
5:A:515:VAL:O	5:A:522:ALA:N	2.51	0.44
5:A:661:TYR:HA	5:A:666:SER:HB3	1.98	0.44
5:A:694:GLN:HG2	6:B:547:LEU:HD12	1.99	0.44
6:B:30:HIS:HD2	15:B:1202:CLA:HBB2	1.82	0.44
15:B:1235:CLA:HBA2	15:B:1235:CLA:C4A	2.45	0.44
16:1:609:CHL:HAA1	4:4:228:THR:CG2	2.46	0.44
2:2:269:SER:C	2:2:271:PRO:HD3	2.38	0.44
3:3:235:LEU:HD13	15:3:601:CLA:HMA1	1.99	0.44
14:4:503:BCR:H403	14:4:503:BCR:C23	2.48	0.44
12:4:501:LUT:H32	15:4:601:CLA:HAB	1.99	0.44
5:A:262:ALA:HB3	5:A:263:PRO:HD3	1.99	0.44
5:A:276:LEU:HD21	5:A:299:LEU:HD12	1.99	0.44
5:A:34:HIS:HA	5:A:40:ALA:HB2	2.00	0.44
5:A:32:PRO:HB2	5:A:48:TRP:HH2	1.83	0.44
6:B:395:PHE:CZ	6:B:409:LEU:HD11	2.52	0.44
9:E:73:LEU:HA	9:E:89:LYS:HA	1.99	0.44
10:F:155:ALA:HB1	10:F:161:ALA:HA	1.98	0.44
14:J:4001:BCR:H351	14:J:4001:BCR:H15C	1.80	0.44
1:1:166:ASP:OD1	1:1:167:PRO:HD2	2.18	0.44
12:1:501:LUT:H31	12:1:501:LUT:H403	1.79	0.44
5:A:261:LEU:O	5:A:261:LEU:HG	2.18	0.44
5:A:75:SER:HG	5:A:181:TYR:HD1	1.63	0.44
6:B:439:VAL:CG1	15:B:1230:CLA:HAC1	2.48	0.44
9:E:91:VAL:HG23	9:E:105:ARG:HB2	2.00	0.44
3:3:121:MET:CG	3:3:243:GLY:HA2	2.48	0.44
15:3:607:CLA:HBA1	15:3:607:CLA:O2D	2.18	0.44
5:A:214:ALA:O	5:A:218:ILE:HG13	2.18	0.44
5:A:682:SER:CB	5:A:730:HIS:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1023:CLA:C1	15:B:1023:CLA:H3A	2.47	0.44
15:B:1216:CLA:HMB2	15:B:1221:CLA:HMA3	2.00	0.44
6:B:456:ILE:HG23	10:F:150:SER:OG	2.18	0.44
1:1:113:PRO:HG2	1:1:120:VAL:CG1	2.47	0.43
4:4:214:THR:O	4:4:218:ILE:HG23	2.18	0.43
15:4:615:CLA:H51	15:4:615:CLA:H11	1.79	0.43
5:A:190:TRP:CZ2	15:A:1108:CLA:HMA1	2.53	0.43
15:B:1219:CLA:HMB3	15:B:1240:CLA:C1D	2.48	0.43
6:B:69:VAL:HG11	6:B:125:TRP:HZ3	1.82	0.43
6:B:134:GLN:O	6:B:138:VAL:HG23	2.18	0.43
6:B:499:LEU:HA	6:B:502:ILE:HG22	1.99	0.43
6:B:585:LEU:HD22	6:B:714:PHE:CD2	2.53	0.43
8:D:100:PHE:CZ	8:D:158:VAL:HG21	2.53	0.43
8:D:190:ARG:HH22	8:D:210:PHE:CB	2.31	0.43
4:4:150:LEU:CD2	10:F:213:GLN:HA	2.47	0.43
1:1:153:TYR:CE2	1:1:174:LYS:HE3	2.53	0.43
16:1:609:CHL:H2A	16:1:609:CHL:O1D	2.17	0.43
4:4:192:VAL:HG12	4:4:194:LEU:HG	2.00	0.43
4:4:205:TYR:CD2	4:4:206:PRO:HD3	2.53	0.43
4:4:264:PHE:CZ	4:4:268:GLY:HA3	2.52	0.43
15:A:1110:CLA:CHA	15:A:1110:CLA:HBA1	2.48	0.43
15:A:1119:CLA:HMA2	15:A:1123:CLA:NC	2.33	0.43
6:B:438:TYR:HD2	15:B:1021:CLA:H203	1.83	0.43
6:B:88:ILE:HG23	6:B:114:VAL:HB	2.00	0.43
15:B:1219:CLA:HBB1	15:B:1219:CLA:HMB1	2.00	0.43
15:B:1235:CLA:H8	15:B:1235:CLA:H52	1.85	0.43
6:B:449:THR:HB	6:B:451:GLU:OE2	2.18	0.43
8:D:209:PRO:O	8:D:210:PHE:HB2	2.18	0.43
2:2:108:VAL:HG11	2:2:169:ARG:HH12	1.80	0.43
15:2:601:CLA:HMD2	16:2:611:CHL:CGA	2.47	0.43
12:3:501:LUT:C28	12:3:501:LUT:H361	2.48	0.43
4:4:281:GLN:HB3	15:4:607:CLA:HMD3	1.99	0.43
15:A:1012:CLA:C4	6:B:439:VAL:HA	2.48	0.43
15:A:1124:CLA:HAA1	15:A:1125:CLA:CAD	2.47	0.43
5:A:443:TRP:HZ3	15:A:1130:CLA:HMC3	1.83	0.43
5:A:728:VAL:HG22	5:A:732:LEU:HD13	2.00	0.43
15:B:1210:CLA:O1A	14:B:4002:BCR:H372	2.17	0.43
15:B:1222:CLA:CBB	15:B:1222:CLA:HMB1	2.48	0.43
15:B:1237:CLA:HBB1	15:B:1237:CLA:HMB1	2.00	0.43
6:B:548:MET:HE3	6:B:554:PHE:CD2	2.53	0.43
6:B:663:MET:N	15:B:1023:CLA:HMC3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:105:TRP:CE3	8:D:107:SER:HB3	2.53	0.43
8:D:138:CYS:O	8:D:142:THR:HG23	2.18	0.43
16:1:609:CHL:HED3	4:4:228:THR:O	2.19	0.43
15:A:1110:CLA:CED	15:A:1111:CLA:HHC	2.35	0.43
5:A:71:ARG:CD	5:A:185:ALA:HB1	2.46	0.43
5:A:352:GLN:HG3	5:A:356:ASN:HD21	1.82	0.43
5:A:531:SER:HB3	5:A:639:ALA:HB3	1.99	0.43
6:B:5:LEU:CD1	6:B:6:PHE:H	2.12	0.43
8:D:79:THR:HG23	8:D:80:PRO:HD2	2.00	0.43
10:F:230:LEU:HG	10:F:231:LEU:HD12	1.99	0.43
15:1:603:CLA:CHD	15:1:615:CLA:HAB	2.49	0.43
1:1:185:MET:SD	15:1:604:CLA:HMC3	2.59	0.43
1:1:83:MET:CE	15:1:601:CLA:CAB	2.96	0.43
2:2:104:GLN:HA	2:2:107:LEU:HD12	2.01	0.43
3:3:143:THR:O	15:3:606:CLA:HED2	2.19	0.43
12:4:501:LUT:H183	15:4:603:CLA:C3B	2.48	0.43
15:4:601:CLA:HBC2	16:4:611:CHL:O1A	2.17	0.43
15:A:1012:CLA:C14	14:J:4001:BCR:H14C	2.48	0.43
5:A:610:PHE:O	5:A:614:MET:HG2	2.19	0.43
5:A:647:ARG:HA	6:B:633:ILE:HG21	2.00	0.43
5:A:598:TRP:CZ3	15:B:1022:CLA:HAB	2.53	0.43
6:B:118:THR:N	15:B:1205:CLA:OBD	2.47	0.43
2:2:134:PRO:HB3	2:2:142:GLU:OE2	2.18	0.43
15:3:605:CLA:HBC2	15:3:605:CLA:CMC	2.46	0.43
4:4:174:MET:HE3	15:4:601:CLA:HMC3	2.00	0.43
5:A:316:TRP:CZ3	15:A:1118:CLA:HAA1	2.54	0.43
6:B:339:LEU:HD21	15:B:1226:CLA:HAB	2.01	0.43
10:F:230:LEU:HD23	10:F:230:LEU:H	1.84	0.43
14:1:505:BCR:H281	15:4:605:CLA:HAC2	2.01	0.43
1:1:56:PHE:O	1:1:57:ASP:C	2.57	0.43
2:2:203:PHE:C	2:2:205:PRO:HD3	2.39	0.43
2:2:204:ASP:OD1	15:2:601:CLA:HBA2	2.18	0.43
2:2:223:VAL:O	2:2:227:ARG:HG3	2.19	0.43
3:3:186:GLN:HB2	3:3:194:GLN:NE2	2.33	0.43
3:3:282:THR:N	15:3:603:CLA:CED	2.82	0.43
14:3:503:BCR:H402	15:3:606:CLA:NB	2.33	0.43
4:4:285:LEU:HG	12:4:501:LUT:H191	2.00	0.43
5:A:25:ASN:OD1	5:A:26:PHE:N	2.51	0.43
6:B:463:TRP:CD2	15:F:1302:CLA:HMA2	2.53	0.43
11:J:1:MET:O	11:J:5:THR:HG23	2.19	0.43
13:2:502:XAT:H203	15:2:605:CLA:HMA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:247:MET:HE1	16:3:604:CHL:HAB	1.99	0.43
3:3:250:MET:HG2	13:3:502:XAT:C12	2.34	0.43
4:4:126:LEU:HD12	4:4:145:TYR:O	2.18	0.43
4:4:166:GLU:HG3	15:4:604:CLA:CHB	2.47	0.43
4:4:273:SER:N	4:4:274:PRO:CD	2.82	0.43
4:4:296:THR:O	4:4:298:ALA:N	2.52	0.43
5:A:241:HIS:CE1	5:A:242:GLU:HG3	2.53	0.43
6:B:662:PHE:CD2	15:B:1022:CLA:HMD2	2.54	0.43
1:1:218:PHE:HB3	15:1:603:CLA:O2A	2.19	0.43
1:1:57:ASP:HB2	15:1:604:CLA:HBA2	2.01	0.43
15:1:612:CLA:HBA1	19:1:811:SQD:C7	2.49	0.43
12:3:501:LUT:H27	12:3:501:LUT:H381	1.86	0.43
4:4:178:VAL:HG21	12:4:501:LUT:C40	2.49	0.43
15:A:1013:CLA:HMD2	6:B:534:ILE:HD13	2.01	0.43
25:A:2001:PQN:H191	25:A:2001:PQN:H211	1.55	0.43
5:A:392:THR:HG23	5:A:607:ILE:HG21	1.99	0.43
6:B:232:ALA:HA	15:B:1213:CLA:HMA2	2.00	0.43
10:F:163:GLU:HA	11:J:38:VAL:HG23	2.00	0.43
15:1:611:CLA:CMC	15:1:611:CLA:HBC2	2.44	0.43
3:3:176:ALA:HB1	14:3:503:BCR:C17	2.48	0.43
14:3:503:BCR:H351	14:3:503:BCR:H15C	1.70	0.43
15:4:615:CLA:HBC1	21:4:811:DGD:C1B	2.49	0.43
5:A:78:PHE:CZ	15:A:1108:CLA:HBB1	2.54	0.43
15:A:1103:CLA:H61	14:A:4003:BCR:H402	2.00	0.43
5:A:358:ALA:HB2	14:A:4005:BCR:H382	1.99	0.43
15:A:1013:CLA:HMD2	6:B:534:ILE:CD1	2.49	0.43
11:J:18:TRP:CZ3	11:J:19:ALA:HB2	2.54	0.43
5:A:119:TRP:CD2	14:J:4002:BCR:HC41	2.53	0.43
5:A:26:PHE:HD2	11:J:4:PHE:HB2	1.84	0.43
15:1:605:CLA:HED1	15:1:612:CLA:H11	2.01	0.42
15:3:612:CLA:CED	15:3:612:CLA:H2A	2.49	0.42
15:4:606:CLA:O2A	16:4:613:CHL:HMD2	2.19	0.42
15:A:1108:CLA:HED2	15:A:1108:CLA:H2A	2.01	0.42
15:A:1110:CLA:CED	15:A:1111:CLA:HMC3	2.48	0.42
15:A:1136:CLA:HMA2	15:A:1137:CLA:HED2	2.00	0.42
5:A:233:ASP:HB3	5:A:236:GLU:HG2	2.01	0.42
5:A:531:SER:O	5:A:535:VAL:HG23	2.18	0.42
5:A:693:TRP:CZ3	25:A:2001:PQN:H2M3	2.54	0.42
5:A:450:PHE:CZ	15:B:1023:CLA:H51	2.54	0.42
15:B:1211:CLA:H43	14:B:4003:BCR:C17	2.49	0.42
15:B:1226:CLA:H2A	15:B:1226:CLA:CED	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1239:CLA:H161	15:B:1239:CLA:H141	1.63	0.42
6:B:664:PHE:CZ	15:B:1239:CLA:HBC3	2.54	0.42
6:B:129:GLY:O	6:B:130:LEU:HG	2.18	0.42
6:B:460:PHE:HB2	15:B:1235:CLA:OBD	2.19	0.42
5:A:577:GLY:HA2	6:B:563:PRO:HD3	2.00	0.42
6:B:453:GLN:NE2	10:F:145:LEU:HD13	2.33	0.42
10:F:176:GLY:O	10:F:177:TYR:C	2.57	0.42
1:1:47:LEU:HA	1:1:50:LEU:HD12	2.01	0.42
1:1:80:ARG:HB3	15:1:601:CLA:HBC3	1.98	0.42
16:2:613:CHL:HAC2	16:2:613:CHL:OMC	2.18	0.42
4:4:150:LEU:HD22	10:F:213:GLN:HA	2.01	0.42
16:1:609:CHL:HAA1	4:4:228:THR:OG1	2.19	0.42
4:4:288:LEU:CD2	15:4:604:CLA:HMC1	2.49	0.42
14:4:503:BCR:H351	14:4:503:BCR:H15C	1.60	0.42
5:A:670:LEU:HD12	15:A:1107:CLA:HAC1	2.00	0.42
5:A:427:LEU:O	5:A:431:ILE:HG13	2.19	0.42
5:A:535:VAL:HG11	5:A:609:HIS:CG	2.54	0.42
5:A:561:ARG:NE	8:D:90:GLY:H	2.17	0.42
6:B:276:HIS:HB3	15:B:1214:CLA:HMB3	2.01	0.42
6:B:345:ILE:O	6:B:349:VAL:HG23	2.19	0.42
8:D:168:HIS:HA	8:D:169:PRO:HA	1.67	0.42
6:B:456:ILE:HD13	10:F:148:LEU:HB2	2.01	0.42
1:1:103:ALA:HA	15:1:606:CLA:CED	2.32	0.42
15:1:605:CLA:HMD2	15:1:612:CLA:C4D	2.50	0.42
2:2:206:MET:O	2:2:208:MET:N	2.52	0.42
15:2:605:CLA:HAC1	15:2:612:CLA:CGA	2.48	0.42
3:3:247:MET:CE	16:3:604:CHL:HAB	2.50	0.42
4:4:264:PHE:HD2	4:4:266:PRO:O	2.02	0.42
5:A:680:ALA:O	15:A:1013:CLA:HAB	2.18	0.42
15:A:1106:CLA:CAD	15:A:1126:CLA:HAA2	2.50	0.42
15:A:1135:CLA:HBB1	15:A:1135:CLA:HMB1	2.01	0.42
15:A:1101:CLA:CGA	25:A:2001:PQN:H222	2.49	0.42
5:A:494:ALA:HB3	5:A:495:PRO:HD3	2.01	0.42
5:A:598:TRP:HZ2	15:B:1023:CLA:ND	2.16	0.42
15:B:1214:CLA:O1D	15:B:1215:CLA:HMA1	2.19	0.42
6:B:235:ALA:HB2	6:B:256:LEU:O	2.19	0.42
6:B:581:VAL:O	6:B:585:LEU:HD13	2.19	0.42
6:B:61:TRP:CG	15:B:1203:CLA:HBC1	2.54	0.42
9:E:90:VAL:HG11	9:E:93:VAL:HG23	2.01	0.42
1:1:183:LEU:HD11	15:1:607:CLA:HHD	2.01	0.42
13:1:502:XAT:H15	13:1:502:XAT:H201	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:107:LEU:HD13	2:2:198:TYR:HE1	1.83	0.42
3:3:154:PRO:CG	3:3:155:PRO:HD3	2.46	0.42
3:3:243:GLY:O	3:3:247:MET:HG3	2.19	0.42
13:3:502:XAT:H31	15:3:605:CLA:HMB1	2.00	0.42
4:4:145:TYR:HD2	15:4:609:CLA:CMC	2.31	0.42
24:A:1011:CL0:H22	6:B:626:TRP:CD1	2.55	0.42
15:A:1103:CLA:HMB1	15:A:1103:CLA:CBB	2.49	0.42
5:A:435:ASP:CG	6:B:678:THR:HG23	2.39	0.42
15:B:1231:CLA:HBA2	15:B:1232:CLA:HMB3	2.01	0.42
6:B:316:LEU:O	6:B:411:ARG:NE	2.52	0.42
15:1:603:CLA:HMB1	15:1:603:CLA:CBB	2.49	0.42
12:2:501:LUT:H201	12:2:501:LUT:H15	1.69	0.42
3:3:147:TRP:HE1	3:3:264:PRO:HD3	1.84	0.42
3:3:153:ILE:O	3:3:153:ILE:HG22	2.20	0.42
3:3:237:LEU:HD12	3:3:238:ASN:N	2.33	0.42
3:3:271:HIS:HE1	15:3:608:CLA:C2C	2.32	0.42
15:A:1012:CLA:HBD	15:A:1012:CLA:HAA2	2.00	0.42
5:A:341:LEU:O	5:A:344:ILE:HB	2.19	0.42
6:B:118:THR:HA	6:B:368:THR:HG22	2.01	0.42
15:B:1239:CLA:H162	15:B:1239:CLA:H193	1.73	0.42
14:B:4004:BCR:H351	14:B:4004:BCR:H15C	1.60	0.42
6:B:547:LEU:HD22	6:B:571:ILE:CD1	2.48	0.42
6:B:17:PRO:HD2	7:C:73:SER:HA	2.01	0.42
14:A:4006:BCR:H383	14:J:4001:BCR:H322	2.01	0.42
14:J:4003:BCR:C8	14:J:4003:BCR:H321	2.50	0.42
1:1:153:TYR:CZ	1:1:174:LYS:HE3	2.55	0.42
2:2:104:GLN:NE2	2:2:169:ARG:HD3	2.34	0.42
15:3:608:CLA:O2D	15:3:608:CLA:HBA2	2.20	0.42
25:A:2001:PQN:H111	25:A:2001:PQN:H2M1	1.75	0.42
25:A:2001:PQN:H261	25:A:2001:PQN:H302	1.83	0.42
5:A:657:VAL:HG13	5:A:658:ILE:HG23	2.00	0.42
6:B:657:VAL:CG2	15:B:1239:CLA:HMB3	2.49	0.42
6:B:341:SER:O	6:B:344:THR:HG22	2.20	0.42
6:B:577:PHE:O	6:B:581:VAL:HG23	2.19	0.42
8:D:109:LYS:O	8:D:110:GLU:C	2.57	0.42
8:D:82:PRO:HB3	8:D:123:MET:HE1	2.01	0.42
4:4:178:VAL:HG23	12:4:501:LUT:H35	2.01	0.42
15:A:1115:CLA:H2A	15:A:1115:CLA:HED2	2.00	0.42
25:A:2001:PQN:H172	14:B:4006:BCR:H331	2.02	0.42
5:A:442:ASN:HD22	5:A:442:ASN:C	2.21	0.42
5:A:459:ASN:ND2	5:A:640:ASN:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:84:ILE:HD13	15:A:1104:CLA:CBC	2.46	0.42
6:B:586:ASN:ND2	15:B:1021:CLA:H43	2.35	0.42
15:B:1217:CLA:HHC	15:B:1217:CLA:HBB1	2.02	0.42
6:B:453:GLN:NE2	6:B:455:LEU:HD11	2.35	0.42
6:B:258:PHE:CE2	6:B:494:TRP:CE3	3.07	0.42
1:1:120:VAL:HG11	15:1:613:CLA:CMD	2.50	0.42
1:1:193:GLY:O	15:1:603:CLA:HMD3	2.19	0.42
2:2:119:GLY:O	2:2:123:THR:HG23	2.20	0.42
2:2:198:TYR:HE2	2:2:219:LYS:HB2	1.85	0.42
3:3:120:ALA:CB	3:3:247:MET:HG2	2.49	0.42
14:3:503:BCR:H292	15:3:606:CLA:C1C	2.50	0.42
15:3:613:CLA:HMB1	15:3:613:CLA:CBB	2.50	0.42
5:A:341:LEU:HD23	5:A:344:ILE:HG13	2.02	0.42
5:A:474:ASP:H	5:A:637:GLN:HE22	1.67	0.42
5:A:81:LEU:HD11	15:A:1111:CLA:HBA2	2.02	0.42
15:A:1012:CLA:CMB	15:B:1021:CLA:H191	2.45	0.42
15:B:1204:CLA:HHC	15:B:1204:CLA:CBB	2.49	0.42
15:B:1215:CLA:CBB	15:B:1215:CLA:HMB1	2.49	0.42
15:B:1224:CLA:CBB	15:B:1224:CLA:HMB1	2.50	0.42
15:B:1229:CLA:H162	15:B:1229:CLA:H202	1.93	0.42
6:B:87:PRO:HA	6:B:122:TYR:HE2	1.85	0.42
10:F:204:VAL:N	10:F:205:PRO:HD2	2.34	0.42
15:A:1121:CLA:HHC	15:A:1121:CLA:HBB1	2.02	0.42
5:A:473:SER:HB3	5:A:637:GLN:NE2	2.35	0.42
5:A:562:LEU:HD11	5:A:580:ARG:HG3	2.02	0.42
15:B:1205:CLA:CBB	15:B:1205:CLA:HMB1	2.49	0.42
6:B:352:HIS:HB3	15:B:1214:CLA:HED2	2.02	0.42
6:B:718:TYR:CZ	15:B:1021:CLA:HED1	2.55	0.42
8:D:105:TRP:HE1	8:D:130:LEU:HD13	1.85	0.42
15:J:1302:CLA:HMD3	14:J:4002:BCR:H311	2.02	0.42
1:1:118:ILE:O	1:1:118:ILE:HG22	2.19	0.42
15:1:605:CLA:HBC1	15:1:612:CLA:CBC	2.49	0.42
16:1:610:CHL:HBD	16:1:610:CHL:CBA	2.50	0.42
3:3:280:LEU:HD22	15:3:603:CLA:C4B	2.50	0.42
3:3:244:ARG:HH11	16:3:604:CHL:CHD	2.33	0.42
24:A:1011:CL0:C3B	15:A:1012:CLA:HED2	2.50	0.42
15:A:1119:CLA:CBB	15:A:1119:CLA:HMB1	2.50	0.42
15:A:1138:CLA:H162	15:A:1138:CLA:H141	1.85	0.42
15:A:1138:CLA:H151	15:A:1139:CLA:H43	2.01	0.42
5:A:334:THR:HA	5:A:429:ARG:NE	2.34	0.42
5:A:338:HIS:HE1	15:A:1122:CLA:ND	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:365:ILE:HG12	5:A:395:MET:HA	2.01	0.42
5:A:436:ALA:HB2	6:B:681:TRP:CH2	2.55	0.42
5:A:69:ILE:O	5:A:73:VAL:HG23	2.19	0.42
15:B:1222:CLA:HBA2	15:B:1236:CLA:HAA1	2.01	0.42
6:B:399:TYR:CD2	6:B:401:PRO:HD3	2.55	0.42
10:F:184:GLN:HE21	10:F:210:LEU:HB3	1.85	0.42
15:3:606:CLA:HBA1	15:3:613:CLA:C2D	2.50	0.41
15:3:612:CLA:HMC1	15:3:613:CLA:HMB1	2.02	0.41
3:3:225:PHE:CD1	20:3:902:CAC:AS	3.33	0.41
4:4:223:PHE:CG	15:4:612:CLA:HMC3	2.55	0.41
4:4:311:HIS:HA	4:4:318:VAL:HG21	2.02	0.41
12:4:501:LUT:H35	12:4:501:LUT:H401	1.83	0.41
21:4:811:DGD:HE62	21:4:811:DGD:O3E	2.20	0.41
5:A:77:HIS:CE1	15:A:1111:CLA:HMD1	2.55	0.41
15:A:1140:CLA:H91	11:J:16:LEU:CD2	2.50	0.41
15:A:1140:CLA:HBC1	14:B:4006:BCR:HC7	2.02	0.41
5:A:580:ARG:O	5:A:580:ARG:HG2	2.20	0.41
5:A:95:GLY:HA3	5:A:148:TRP:CZ3	2.55	0.41
15:B:1228:CLA:H62	15:B:1228:CLA:H92	1.75	0.41
6:B:388:PHE:HA	14:B:4005:BCR:H382	2.01	0.41
8:D:95:ALA:HA	8:D:99:GLU:O	2.20	0.41
15:3:608:CLA:HBB1	15:3:608:CLA:HHC	2.03	0.41
5:A:516:ALA:HB2	5:A:521:VAL:HG12	2.02	0.41
6:B:63:SER:OG	6:B:140:SER:O	2.27	0.41
6:B:395:PHE:HZ	6:B:409:LEU:HD11	1.84	0.41
1:1:206:LEU:HD12	12:1:501:LUT:H22	2.02	0.41
2:2:228:LEU:CD2	15:2:602:CLA:HAA1	2.50	0.41
12:2:501:LUT:H393	15:2:602:CLA:HBA2	2.02	0.41
15:4:602:CLA:HBC3	15:4:602:CLA:HHD	2.02	0.41
5:A:85:LEU:CB	5:A:170:ALA:HB2	2.50	0.41
6:B:277:HIS:HB2	15:B:1214:CLA:CHB	2.50	0.41
15:B:1222:CLA:HMA1	14:B:4005:BCR:H14C	2.01	0.41
6:B:659:ALA:HB1	15:B:1023:CLA:HAB	2.02	0.41
12:2:501:LUT:H191	12:2:501:LUT:H11	1.67	0.41
15:4:601:CLA:HBA1	15:4:601:CLA:NA	2.30	0.41
5:A:299:LEU:HD21	15:A:1113:CLA:HMC1	2.01	0.41
15:A:1124:CLA:H12	15:A:1135:CLA:HMA1	2.02	0.41
15:A:1139:CLA:H52	15:A:1139:CLA:H11	1.88	0.41
5:A:129:GLY:N	5:A:137:GLY:O	2.53	0.41
5:A:74:PHE:HB2	5:A:191:PHE:HE1	1.86	0.41
5:A:441:LEU:HB3	5:A:548:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:687:PHE:HE1	6:B:666:ILE:HG13	1.86	0.41
15:B:1232:CLA:HMB1	15:B:1232:CLA:HBB1	2.02	0.41
6:B:426:VAL:O	6:B:430:LEU:HD23	2.20	0.41
14:A:4007:BCR:HC31	6:B:649:TRP:CZ3	2.55	0.41
10:F:148:LEU:HD13	10:F:163:GLU:OE1	2.21	0.41
15:1:615:CLA:HED2	15:1:615:CLA:H2A	2.02	0.41
2:2:203:PHE:HB2	15:2:601:CLA:OBD	2.21	0.41
2:2:199:PRO:HD2	15:2:601:CLA:O2D	2.21	0.41
3:3:110:GLN:O	3:3:113:GLU:HG2	2.19	0.41
3:3:158:VAL:HG13	3:3:158:VAL:O	2.20	0.41
3:3:122:LEU:HD12	15:3:606:CLA:HMC2	2.02	0.41
3:3:169:LEU:CD1	15:3:613:CLA:HMD3	2.50	0.41
5:A:679:TRP:CG	24:A:1011:CL0:H5	2.56	0.41
15:A:1125:CLA:HBB1	15:A:1125:CLA:CHC	2.41	0.41
5:A:282:LEU:HA	5:A:290:TRP:CZ3	2.56	0.41
14:A:4007:BCR:HC31	6:B:649:TRP:HZ3	1.85	0.41
5:A:479:LEU:HB2	5:A:530:THR:HG23	2.01	0.41
6:B:175:ARG:HB2	15:B:1210:CLA:CBC	2.50	0.41
6:B:175:ARG:HD3	15:B:1210:CLA:HBC2	2.03	0.41
3:3:111:TYR:CD1	3:3:213:ALA:HA	2.55	0.41
3:3:279:ASN:HB3	3:3:280:LEU:H	1.79	0.41
4:4:205:TYR:N	4:4:206:PRO:CD	2.83	0.41
4:4:272:THR:O	4:4:272:THR:HG23	2.20	0.41
5:A:516:ALA:HA	5:A:522:ALA:H	1.86	0.41
5:A:602:SER:O	5:A:606:VAL:HG23	2.21	0.41
5:A:653:GLN:O	5:A:746:ARG:HD3	2.20	0.41
15:B:1234:CLA:CBB	15:B:1234:CLA:HHC	2.50	0.41
6:B:423:LEU:HD21	15:B:1236:CLA:CMB	2.50	0.41
6:B:191:TRP:NE1	6:B:195:LEU:HD11	2.35	0.41
6:B:255:ILE:HG13	6:B:256:LEU:N	2.36	0.41
1:1:103:ALA:HB3	1:1:104:PRO:CD	2.51	0.41
1:1:130:VAL:HA	1:1:133:VAL:HG22	2.03	0.41
1:1:217:ASN:CG	15:1:608:CLA:HED1	2.41	0.41
14:3:504:BCR:H313	15:3:612:CLA:H43	2.02	0.41
4:4:226:VAL:HG11	16:4:611:CHL:C1B	2.51	0.41
15:A:1013:CLA:H41	15:A:1013:CLA:H61	1.67	0.41
15:A:1110:CLA:HED2	15:A:1110:CLA:C4D	2.49	0.41
15:A:1111:CLA:C2	15:A:1111:CLA:HMA2	2.50	0.41
15:A:1124:CLA:H2	15:A:1125:CLA:CED	2.46	0.41
5:A:447:PHE:O	5:A:451:HIS:ND1	2.44	0.41
5:A:603:LEU:O	5:A:607:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:63:THR:HG23	5:A:65:ASP:H	1.86	0.41
15:B:1205:CLA:H2A	15:B:1205:CLA:O2D	2.21	0.41
15:B:1222:CLA:HBB1	15:B:1222:CLA:HMB1	2.01	0.41
15:B:1239:CLA:HHC	15:B:1239:CLA:CBB	2.50	0.41
15:B:1211:CLA:H11	14:B:4003:BCR:H21C	2.02	0.41
6:B:404:ASN:OD1	6:B:407:ASN:ND2	2.53	0.41
6:B:312:PRO:HG2	17:B:5001:LHG:HC31	2.03	0.41
11:J:2:LYS:HE2	11:J:2:LYS:HB3	1.87	0.41
16:1:610:CHL:HBC2	15:1:613:CLA:CMC	2.50	0.41
1:1:72:ARG:HE	1:1:152:LEU:CD1	2.34	0.41
16:2:609:CHL:C2D	14:3:503:BCR:H312	2.51	0.41
16:2:609:CHL:HMD2	14:3:503:BCR:HC42	2.02	0.41
13:3:502:XAT:C28	13:3:502:XAT:H381	2.31	0.41
12:4:501:LUT:H183	15:4:603:CLA:C4B	2.51	0.41
24:A:1011:CL0:H10	24:A:1011:CL0:CMA	2.41	0.41
6:B:429:PHE:CD2	15:B:1235:CLA:HAB	2.55	0.41
6:B:196:VAL:HG23	6:B:197:HIS:ND1	2.35	0.41
6:B:388:PHE:CG	6:B:535:LEU:HD13	2.55	0.41
6:B:55:LEU:O	6:B:59:PHE:HD2	2.04	0.41
10:F:186:ILE:O	10:F:190:LYS:HG2	2.20	0.41
13:1:502:XAT:H191	13:1:502:XAT:H11	1.92	0.41
13:1:502:XAT:H391	13:1:502:XAT:H31	1.82	0.41
2:2:110:CYS:CB	2:2:226:GLY:HA3	2.49	0.41
15:4:604:CLA:H3A	15:4:604:CLA:HBA2	1.30	0.41
16:4:613:CHL:HAC2	16:4:613:CHL:OMC	2.19	0.41
5:A:673:LEU:HB3	15:A:1012:CLA:C2	2.50	0.41
15:A:1138:CLA:H143	15:A:1139:CLA:H43	2.03	0.41
5:A:325:ILE:HG23	5:A:329:HIS:HE1	1.85	0.41
14:A:4006:BCR:H351	14:A:4006:BCR:H15C	1.86	0.41
5:A:446:ILE:HG23	5:A:450:PHE:CE2	2.56	0.41
5:A:665:LEU:HD22	5:A:668:TYR:CE2	2.56	0.41
6:B:102:VAL:HA	6:B:113:PRO:HG3	2.03	0.41
15:B:1222:CLA:CGA	15:B:1234:CLA:HMA1	2.51	0.41
6:B:206:GLN:HB3	6:B:208:VAL:HG23	2.02	0.41
5:A:578:PRO:HD3	6:B:562:GLY:HA2	2.03	0.41
6:B:5:LEU:HD12	6:B:21:ARG:NH1	2.36	0.41
15:A:1139:CLA:H41	15:F:1301:CLA:HMD3	2.03	0.41
15:4:615:CLA:HED3	15:J:1302:CLA:C3	2.51	0.41
11:J:21:PHE:HE1	14:J:4003:BCR:HC21	1.85	0.41
15:J:1302:CLA:HAC1	14:J:4002:BCR:H10C	2.02	0.41
14:A:4005:BCR:H331	14:A:4005:BCR:C8	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:509:THR:HA	5:A:525:PRO:HA	2.03	0.41
5:A:644:GLY:HA2	5:A:647:ARG:HB3	2.03	0.41
15:B:1203:CLA:HMC2	14:B:4002:BCR:H401	2.03	0.41
15:B:1230:CLA:HBA2	14:B:4006:BCR:H271	2.01	0.41
15:B:1239:CLA:O1A	25:B:2002:PQN:H271	2.20	0.41
6:B:131:ARG:HD2	6:B:207:HIS:ND1	2.35	0.41
6:B:263:HIS:HD1	6:B:266:THR:H	1.68	0.41
5:A:702:TRP:CH2	6:B:418:ALA:HB2	2.56	0.41
7:C:55:GLU:OE2	7:C:66:ARG:HA	2.21	0.41
2:2:232:ALA:HB2	12:2:501:LUT:H392	2.02	0.41
16:2:613:CHL:HAA2	16:2:613:CHL:CBD	2.50	0.41
3:3:152:VAL:HG23	15:3:610:CLA:C1D	2.51	0.41
3:3:234:LYS:O	3:3:237:LEU:HG	2.22	0.41
3:3:271:HIS:CE1	15:3:608:CLA:C2C	3.04	0.41
15:4:604:CLA:CBB	15:4:604:CLA:HHC	2.51	0.41
15:A:1109:CLA:CBD	15:A:1109:CLA:HBA1	2.51	0.41
5:A:483:PHE:HD2	15:A:1136:CLA:HMD2	1.86	0.41
14:A:4002:BCR:C34	14:A:4002:BCR:C6	2.99	0.41
5:A:442:ASN:ND2	15:B:1023:CLA:HED1	2.36	0.41
5:A:521:VAL:O	5:A:521:VAL:HG23	2.21	0.41
5:A:679:TRP:CH2	5:A:683:LEU:HD11	2.56	0.41
15:B:1225:CLA:HBB1	15:B:1225:CLA:CHC	2.42	0.41
15:B:1240:CLA:CBB	15:B:1240:CLA:HMB1	2.50	0.41
6:B:341:SER:HA	6:B:344:THR:HG22	2.03	0.41
6:B:601:THR:HG21	6:B:610:PHE:HB2	2.03	0.41
6:B:441:ASN:CB	6:B:616:TYR:HB3	2.51	0.41
8:D:141:LEU:CD1	8:D:145:LEU:HD11	2.51	0.41
5:A:130:ASP:OD2	10:F:105:ARG:HD3	2.21	0.41
10:F:166:ILE:CD1	10:F:167:PRO:HD3	2.50	0.41
15:4:604:CLA:H43	10:F:219:LEU:HD22	2.03	0.41
12:1:501:LUT:H193	15:1:602:CLA:HMC2	2.02	0.40
16:2:609:CHL:CED	3:3:182:LEU:HB3	2.52	0.40
5:A:35:PHE:HB2	5:A:62:HIS:CG	2.56	0.40
5:A:483:PHE:O	5:A:487:ILE:HG12	2.21	0.40
5:A:526:ILE:HG12	5:A:618:VAL:CG2	2.51	0.40
5:A:669:GLY:O	5:A:672:PHE:HB3	2.21	0.40
5:A:675:ALA:CB	5:A:737:ALA:HB3	2.51	0.40
15:B:1021:CLA:CAB	15:B:1022:CLA:HED3	2.51	0.40
6:B:374:THR:HG22	15:B:1224:CLA:CAB	2.51	0.40
6:B:30:HIS:HD2	15:B:1202:CLA:CBB	2.33	0.40
15:B:1227:CLA:HBC2	14:B:4004:BCR:H393	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:15:THR:HG22	7:C:28:MET:HE2	2.02	0.40
9:E:94:ASP:HB3	9:E:101:PRO:HA	2.03	0.40
4:4:158:ARG:NE	10:F:223:GLN:HG3	2.36	0.40
1:1:120:VAL:HG11	15:1:613:CLA:HMD2	2.04	0.40
1:1:218:PHE:CE2	15:1:615:CLA:HMB3	2.57	0.40
15:1:611:CLA:CBB	15:1:611:CLA:HMB1	2.50	0.40
15:3:601:CLA:HHC	15:3:601:CLA:CBB	2.51	0.40
14:4:505:BCR:C8	14:4:505:BCR:H321	2.51	0.40
15:A:1104:CLA:H61	15:A:1104:CLA:H93	1.89	0.40
5:A:448:LEU:HD21	15:A:1136:CLA:CBB	2.51	0.40
5:A:234:PRO:HA	5:A:237:ILE:HD12	2.04	0.40
6:B:273:ASP:HB3	15:B:1214:CLA:HMA1	2.03	0.40
14:B:4003:BCR:H15C	14:B:4003:BCR:H351	1.72	0.40
6:B:54:GLN:CD	15:B:1202:CLA:HMA1	2.41	0.40
11:J:10:THR:CB	11:J:12:PRO:HD2	2.51	0.40
14:J:4003:BCR:H351	14:J:4003:BCR:H15C	1.91	0.40
3:3:153:ILE:C	3:3:155:PRO:HD2	2.41	0.40
5:A:214:ALA:HB1	5:A:299:LEU:HG	2.03	0.40
5:A:459:ASN:OD1	5:A:472:PHE:HB2	2.21	0.40
19:1:811:SQD:H102	15:B:1219:CLA:CHB	2.52	0.40
6:B:70:ALA:HB2	6:B:136:LEU:HB2	2.03	0.40
6:B:193:GLY:HA2	6:B:196:VAL:HG22	2.03	0.40
6:B:47:ILE:HG22	6:B:51:HIS:HE1	1.87	0.40
6:B:592:THR:HB	6:B:722:TYR:OH	2.21	0.40
15:J:1302:CLA:CAC	14:J:4002:BCR:H10C	2.51	0.40
1:1:218:PHE:O	1:1:224:SER:HB2	2.22	0.40
14:1:505:BCR:H10C	14:4:505:BCR:C20	2.51	0.40
1:1:70:ARG:CZ	19:1:811:SQD:O49	2.70	0.40
2:2:221:LYS:CD	15:2:602:CLA:HMC2	2.51	0.40
13:4:502:XAT:H391	13:4:502:XAT:H31	1.67	0.40
16:4:611:CHL:H2A	16:4:611:CHL:O2D	2.21	0.40
5:A:393:HIS:O	5:A:397:ILE:HG12	2.21	0.40
5:A:51:ASN:ND2	17:A:5002:LHG:O2	2.51	0.40
5:A:500:PRO:HG2	15:A:1134:CLA:HMD3	2.02	0.40
5:A:526:ILE:HG12	5:A:618:VAL:HG22	2.03	0.40
6:B:378:TYR:HB3	15:B:1224:CLA:HMC3	2.04	0.40
8:D:142:THR:HG22	8:D:153:PRO:HG2	2.03	0.40
9:E:89:LYS:NZ	9:E:105:ARG:HD3	2.36	0.40
10:F:239:VAL:HG13	10:F:240:SER:N	2.37	0.40
1:1:114:THR:HG22	1:1:119:GLU:HA	2.04	0.40
15:1:603:CLA:CHB	15:1:608:CLA:HMD3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:240:ILE:HG22	3:3:244:ARG:NH2	2.37	0.40
4:4:145:TYR:HD2	15:4:609:CLA:HMC3	1.86	0.40
4:4:181:LEU:HD22	4:4:305:ILE:HD11	2.03	0.40
4:4:129:PRO:HG3	15:4:609:CLA:HMD3	2.04	0.40
2:2:271:PRO:HB2	15:A:1114:CLA:O1D	2.22	0.40
15:A:1117:CLA:CBB	15:A:1117:CLA:HMB1	2.51	0.40
5:A:249:ILE:O	5:A:253:LEU:HD23	2.22	0.40
5:A:361:GLY:HA2	5:A:398:GLY:HA2	2.03	0.40
14:A:4002:BCR:H15C	14:A:4002:BCR:H351	1.89	0.40
5:A:539:HIS:CG	5:A:606:VAL:HG22	2.57	0.40
5:A:676:HIS:HB3	15:A:1012:CLA:HBD	2.04	0.40
5:A:700:ILE:HG22	5:A:704:HIS:HE1	1.87	0.40
15:B:1231:CLA:H11	15:B:1231:CLA:H52	1.93	0.40
6:B:560:CYS:HB2	6:B:568:THR:O	2.21	0.40
6:B:531:THR:OG1	6:B:583:TRP:HB3	2.22	0.40
6:B:77:GLN:O	6:B:85:VAL:HG11	2.21	0.40
6:B:93:TRP:O	6:B:95:PRO:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:168:LYS:NZ	23:4:831:GSH:O31[2_555]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
2	2	209/211 (99%)	194 (93%)	15 (7%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	209/211 (99%)	184 (88%)	25 (12%)	0	100	100
5	A	737/739 (100%)	702 (95%)	35 (5%)	0	100	100
6	B	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	D	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	37
9	E	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
10	F	161/163 (99%)	145 (90%)	16 (10%)	0	100	100
11	J	39/41 (95%)	30 (77%)	9 (23%)	0	100	100
All	All	2768/2790 (99%)	2588 (94%)	178 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	175	PRO
8	D	174	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	151/151 (100%)	151 (100%)	0	100	100
2	2	169/169 (100%)	169 (100%)	0	100	100
3	3	160/160 (100%)	159 (99%)	1 (1%)	86	94
4	4	169/169 (100%)	166 (98%)	3 (2%)	59	79
5	A	598/598 (100%)	594 (99%)	4 (1%)	84	92
6	B	593/593 (100%)	589 (99%)	4 (1%)	84	92
7	C	68/68 (100%)	68 (100%)	0	100	100
8	D	122/122 (100%)	121 (99%)	1 (1%)	81	91
9	E	57/57 (100%)	56 (98%)	1 (2%)	59	79
10	F	136/136 (100%)	134 (98%)	2 (2%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	36/36 (100%)	36 (100%)	0	100	100
All	All	2259/2259 (100%)	2243 (99%)	16 (1%)	84	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	221	ASN
4	4	128	TYR
4	4	163	ARG
4	4	300	ASN
5	A	44	ASN
5	A	432	ARG
5	A	442	ASN
5	A	580	ARG
6	B	293	ARG
6	B	301	ARG
6	B	586	ASN
6	B	641	MET
8	D	189	MET
9	E	70	ARG
10	F	105	ARG
10	F	125	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	221	ASN
2	2	239	GLN
2	2	250	ASN
3	3	178	GLN
3	3	267	ASN
3	3	271	HIS
3	3	279	ASN
4	4	203	GLN
4	4	281	GLN
5	A	653	GLN
6	B	445	GLN
6	B	453	GLN
10	F	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 203 ligands modelled in this entry, 1 is monoatomic - leaving 202 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	CLA	4	604	4	43,57,73	1.58	9 (20%)	46,93,113	2.10	9 (19%)
15	CLA	A	1124	-	43,57,73	1.50	8 (18%)	46,93,113	2.12	10 (21%)
15	CLA	A	1133	-	43,57,73	1.56	8 (18%)	46,93,113	2.01	8 (17%)
14	BCR	B	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.60	20 (35%)
15	CLA	2	608	-	43,57,73	1.53	8 (18%)	46,93,113	2.16	10 (21%)
13	XAT	3	502	-	39,47,47	0.67	1 (2%)	54,74,74	1.92	14 (25%)
15	CLA	2	601	-	43,57,73	1.46	7 (16%)	46,93,113	1.98	10 (21%)
15	CLA	B	1218	-	43,57,73	1.54	9 (20%)	46,93,113	2.09	9 (19%)
15	CLA	A	1119	-	43,57,73	1.56	7 (16%)	46,93,113	2.08	9 (19%)
14	BCR	B	4004	-	41,41,41	1.78	4 (9%)	56,56,56	4.46	15 (26%)
15	CLA	A	1127	-	43,57,73	1.58	8 (18%)	46,93,113	2.16	10 (21%)
15	CLA	A	1134	-	43,57,73	1.53	8 (18%)	46,93,113	2.13	9 (19%)
15	CLA	A	1130	-	49,63,73	1.47	7 (14%)	55,101,113	1.99	9 (16%)
12	LUT	4	501	-	42,43,43	2.39	2 (4%)	51,60,60	1.92	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	4	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.47	18 (32%)
15	CLA	B	1205	-	43,57,73	1.53	9 (20%)	46,93,113	2.16	9 (19%)
15	CLA	A	1117	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	8 (17%)
15	CLA	A	1013	-	59,73,73	1.35	7 (11%)	67,113,113	1.83	11 (16%)
15	CLA	B	1213	-	43,57,73	1.43	8 (18%)	46,93,113	2.00	10 (21%)
15	CLA	4	603	-	43,57,73	1.55	8 (18%)	46,93,113	2.02	9 (19%)
15	CLA	3	612	-	49,63,73	1.39	8 (16%)	55,101,113	1.96	10 (18%)
19	SQD	1	811	-	39,40,54	0.89	0	48,51,65	0.99	3 (6%)
15	CLA	1	601	-	43,57,73	1.49	8 (18%)	46,93,113	2.01	9 (19%)
15	CLA	B	1227	-	36,53,73	1.78	8 (22%)	39,89,113	2.13	8 (20%)
15	CLA	A	1108	-	40,54,73	1.65	8 (20%)	44,90,113	2.04	9 (20%)
15	CLA	B	1214	-	43,57,73	1.55	9 (20%)	46,93,113	2.08	10 (21%)
21	DGD	4	811	-	46,46,67	0.90	2 (4%)	60,60,81	0.98	3 (5%)
15	CLA	B	1229	-	59,73,73	1.40	6 (10%)	67,113,113	1.85	11 (16%)
15	CLA	3	607	-	44,58,73	1.53	8 (18%)	49,95,113	2.04	10 (20%)
25	PQN	B	2002	-	34,34,34	0.44	0	42,45,45	1.17	3 (7%)
15	CLA	B	1202	-	43,57,73	1.53	6 (13%)	46,93,113	2.08	8 (17%)
21	DGD	B	5002	-	39,39,67	0.93	2 (5%)	53,53,81	1.00	3 (5%)
15	CLA	B	1209	-	40,54,73	1.60	8 (20%)	44,90,113	1.95	7 (15%)
16	CHL	4	610	-	41,55,74	0.92	3 (7%)	41,91,114	1.45	10 (24%)
15	CLA	4	607	-	43,57,73	1.57	8 (18%)	46,93,113	2.01	10 (21%)
15	CLA	B	1204	-	43,57,73	1.56	8 (18%)	46,93,113	2.04	9 (19%)
15	CLA	A	1136	-	43,57,73	1.53	7 (16%)	46,93,113	2.10	8 (17%)
15	CLA	B	1211	-	43,57,73	1.53	9 (20%)	46,93,113	2.09	7 (15%)
15	CLA	A	1106	-	59,73,73	1.33	8 (13%)	67,113,113	1.86	9 (13%)
15	CLA	A	1113	-	36,53,73	1.68	9 (25%)	39,89,113	2.02	7 (17%)
14	BCR	J	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.39	17 (30%)
15	CLA	4	608	-	40,54,73	1.56	8 (20%)	44,90,113	1.98	6 (13%)
15	CLA	F	1301	-	41,55,73	1.59	6 (14%)	45,91,113	2.08	8 (17%)
23	GSH	4	831	-	12,19,19	2.42	4 (33%)	15,24,24	1.73	2 (13%)
15	CLA	2	602	-	43,57,73	1.58	7 (16%)	46,93,113	2.14	9 (19%)
16	CHL	4	613	-	44,58,74	0.99	3 (6%)	43,94,114	1.52	11 (25%)
26	SF4	A	3001	5,6	0,12,12	0.00	-	-	-	-
15	CLA	2	607	-	43,57,73	1.57	7 (16%)	46,93,113	2.12	8 (17%)
15	CLA	B	1230	-	43,57,73	1.57	8 (18%)	46,93,113	2.20	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	1	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.54	21 (37%)
15	CLA	3	613	-	40,54,73	1.62	6 (15%)	44,90,113	1.92	6 (13%)
15	CLA	1	604	1	43,57,73	1.53	8 (18%)	46,93,113	2.13	11 (23%)
14	BCR	J	4002	-	41,41,41	1.82	5 (12%)	56,56,56	4.52	21 (37%)
15	CLA	2	604	-	43,57,73	1.48	7 (16%)	46,93,113	2.04	10 (21%)
18	LMG	2	803	-	15,16,55	0.51	0	20,22,63	0.54	0
14	BCR	B	4006	-	41,41,41	1.89	4 (9%)	56,56,56	4.41	15 (26%)
15	CLA	A	1138	-	59,73,73	1.33	7 (11%)	67,113,113	1.81	9 (13%)
20	CAC	4	902	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	A	1128	-	43,57,73	1.56	8 (18%)	46,93,113	2.15	8 (17%)
15	CLA	J	1302	-	43,57,73	1.55	7 (16%)	46,93,113	2.02	7 (15%)
15	CLA	B	1231	6	54,68,73	1.37	6 (11%)	61,107,113	1.88	10 (16%)
14	BCR	4	505	-	41,41,41	1.87	4 (9%)	56,56,56	4.52	18 (32%)
13	XAT	4	502	-	39,47,47	0.73	0	54,74,74	1.90	13 (24%)
15	CLA	A	1118	-	43,57,73	1.53	9 (20%)	46,93,113	2.09	8 (17%)
15	CLA	4	615	-	49,63,73	1.43	6 (12%)	55,101,113	1.91	9 (16%)
15	CLA	A	1129	-	42,56,73	1.55	7 (16%)	46,92,113	2.01	9 (19%)
18	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.19	3 (9%)
15	CLA	B	1215	-	43,57,73	1.66	7 (16%)	46,93,113	2.28	9 (19%)
15	CLA	4	605	-	43,57,73	1.64	7 (16%)	46,93,113	2.15	9 (19%)
15	CLA	B	1224	-	43,57,73	1.53	8 (18%)	46,93,113	2.04	9 (19%)
15	CLA	A	1104	-	54,68,73	1.34	8 (14%)	61,107,113	1.99	10 (16%)
20	CAC	1	902	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	2	612	-	43,57,73	1.58	8 (18%)	46,93,113	2.12	8 (17%)
15	CLA	A	1115	-	43,57,73	1.58	8 (18%)	46,93,113	2.16	9 (19%)
15	CLA	3	605	-	40,54,73	1.56	8 (20%)	44,90,113	1.87	6 (13%)
15	CLA	A	1114	-	40,54,73	1.58	9 (22%)	44,90,113	1.98	6 (13%)
15	CLA	B	1022	-	44,58,73	1.49	7 (15%)	49,95,113	2.10	12 (24%)
15	CLA	3	615	-	40,54,73	1.61	7 (17%)	44,90,113	1.96	7 (15%)
15	CLA	4	601	4	43,57,73	1.47	6 (13%)	46,93,113	2.08	12 (26%)
15	CLA	B	1203	-	43,57,73	1.53	7 (16%)	46,93,113	2.08	7 (15%)
14	BCR	1	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.53	16 (28%)
15	CLA	1	613	-	36,53,73	1.61	8 (22%)	39,89,113	2.05	7 (17%)
12	LUT	1	501	-	42,43,43	2.44	1 (2%)	51,60,60	4.93	27 (52%)
15	CLA	B	1207	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1220	-	49,63,73	1.47	7 (14%)	55,101,113	1.95	11 (20%)
18	LMG	1	803	-	23,23,55	0.58	0	31,31,63	1.36	2 (6%)
15	CLA	3	610	-	43,57,73	1.53	8 (18%)	46,93,113	1.98	9 (19%)
15	CLA	B	1236	-	43,57,73	1.50	8 (18%)	46,93,113	2.14	10 (21%)
15	CLA	A	1111	-	43,57,73	1.49	7 (16%)	46,93,113	2.17	11 (23%)
17	LHG	B	5001	15	20,20,48	0.64	0	23,26,54	1.43	2 (8%)
15	CLA	4	606	-	43,57,73	1.57	8 (18%)	46,93,113	2.08	8 (17%)
15	CLA	B	1206	6	43,57,73	1.53	8 (18%)	46,93,113	2.10	9 (19%)
15	CLA	1	602	-	40,54,73	1.57	9 (22%)	44,90,113	1.93	7 (15%)
15	CLA	B	1226	-	43,57,73	1.53	8 (18%)	46,93,113	2.19	9 (19%)
15	CLA	B	1239	-	59,73,73	1.32	7 (11%)	67,113,113	1.81	9 (13%)
15	CLA	B	1216	-	43,57,73	1.47	7 (16%)	46,93,113	2.07	9 (19%)
17	LHG	1	801	15	22,22,48	0.56	0	25,28,54	1.33	3 (12%)
15	CLA	A	1012	-	54,68,73	1.44	8 (14%)	61,107,113	1.95	12 (19%)
15	CLA	A	1110	-	43,57,73	1.49	8 (18%)	46,93,113	2.10	9 (19%)
14	BCR	2	503	-	41,41,41	1.87	4 (9%)	56,56,56	4.50	17 (30%)
15	CLA	A	1109	15	43,57,73	1.52	8 (18%)	46,93,113	2.11	9 (19%)
15	CLA	A	1132	-	43,57,73	1.52	9 (20%)	46,93,113	2.13	9 (19%)
16	CHL	2	609	2	44,58,74	0.98	3 (6%)	43,94,114	1.40	10 (23%)
15	CLA	B	1240	17	59,73,73	1.34	7 (11%)	67,113,113	1.79	10 (14%)
15	CLA	B	1217	-	40,54,73	1.59	8 (20%)	44,90,113	1.90	7 (15%)
21	DGD	2	811	-	48,48,67	0.94	3 (6%)	62,62,81	1.06	3 (4%)
22	LMT	2	821	-	24,24,36	1.34	5 (20%)	35,35,47	1.04	2 (5%)
15	CLA	A	1122	-	43,57,73	1.52	8 (18%)	46,93,113	2.07	8 (17%)
15	CLA	B	1221	-	43,57,73	1.54	7 (16%)	46,93,113	2.15	10 (21%)
15	CLA	1	606	-	36,53,73	1.65	6 (16%)	39,89,113	2.12	8 (20%)
15	CLA	B	1021	-	59,73,73	1.36	8 (13%)	67,113,113	1.86	11 (16%)
14	BCR	B	4002	-	41,41,41	1.90	4 (9%)	56,56,56	4.37	17 (30%)
15	CLA	4	612	-	43,57,73	1.59	9 (20%)	46,93,113	2.13	10 (21%)
15	CLA	1	611	-	43,57,73	1.56	7 (16%)	46,93,113	2.06	9 (19%)
20	CAC	3	902	-	0,4,4	0.00	-	0,6,6	0.00	-
21	DGD	J	5001	-	29,29,67	0.61	0	41,41,81	0.60	0
15	CLA	B	1235	-	54,68,73	1.35	9 (16%)	61,107,113	1.89	10 (16%)
15	CLA	3	601	-	43,57,73	1.61	7 (16%)	46,93,113	2.20	9 (19%)
13	XAT	2	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1223	-	44,58,73	1.63	8 (18%)	49,95,113	2.18	11 (22%)
15	CLA	A	1107	5	43,57,73	1.54	7 (16%)	46,93,113	2.08	8 (17%)
20	CAC	4	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	A	1120	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	9 (19%)
15	CLA	A	1141	-	44,58,73	1.52	7 (15%)	49,95,113	2.07	9 (18%)
15	CLA	B	1228	-	54,68,73	1.32	7 (12%)	61,107,113	1.82	10 (16%)
18	LMG	1	802	-	36,36,55	0.73	1 (2%)	44,44,63	1.19	4 (9%)
15	CLA	4	602	-	43,57,73	1.50	7 (16%)	46,93,113	2.03	8 (17%)
16	CHL	1	610	-	41,55,74	1.07	2 (4%)	41,91,114	1.50	11 (26%)
15	CLA	2	605	-	59,73,73	1.34	8 (13%)	67,113,113	1.89	12 (17%)
15	CLA	B	1222	-	43,57,73	1.58	8 (18%)	46,93,113	2.15	8 (17%)
26	SF4	C	3002	7	0,12,12	0.00	-	-	-	-
20	CAC	1	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	1	612	-	53,67,73	1.41	8 (15%)	59,105,113	1.89	8 (13%)
15	CLA	2	615	2	44,58,73	1.50	9 (20%)	49,95,113	2.05	9 (18%)
14	BCR	F	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.56	19 (33%)
15	CLA	A	1140	-	49,63,73	1.47	9 (18%)	55,101,113	1.95	8 (14%)
14	BCR	A	4005	-	41,41,41	4.26	5 (12%)	56,56,56	4.55	21 (37%)
15	CLA	A	1123	-	42,56,73	1.59	8 (19%)	46,92,113	2.01	9 (19%)
17	LHG	2	801	-	20,20,48	0.62	0	23,26,54	1.48	2 (8%)
15	CLA	B	1023	-	54,68,73	1.36	8 (14%)	61,107,113	1.80	11 (18%)
15	CLA	B	1210	-	43,57,73	1.47	6 (13%)	46,93,113	2.12	8 (17%)
15	CLA	1	615	-	59,73,73	1.32	8 (13%)	67,113,113	1.84	9 (13%)
14	BCR	A	4004	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	15 (26%)
15	CLA	4	609	4	43,57,73	1.52	6 (13%)	46,93,113	2.19	10 (21%)
15	CLA	A	1116	-	43,57,73	1.51	8 (18%)	46,93,113	2.12	8 (17%)
14	BCR	B	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	17 (30%)
14	BCR	J	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.42	14 (25%)
14	BCR	A	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.33	17 (30%)
14	BCR	3	504	-	41,41,41	1.87	4 (9%)	56,56,56	4.57	17 (30%)
15	CLA	B	1234	-	43,57,73	1.53	7 (16%)	46,93,113	2.10	10 (21%)
14	BCR	3	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.34	17 (30%)
25	PQN	A	2001	-	34,34,34	0.49	0	42,45,45	1.17	3 (7%)
16	CHL	2	611	-	42,56,74	1.01	2 (4%)	42,92,114	1.42	12 (28%)
17	LHG	A	5001	-	15,15,48	0.75	1 (6%)	16,19,54	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1219	-	43,57,73	1.53	9 (20%)	46,93,113	2.06	9 (19%)
14	BCR	A	4007	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	18 (32%)
15	CLA	A	1126	-	43,57,73	1.59	6 (13%)	46,93,113	2.17	8 (17%)
15	CLA	2	603	-	40,54,73	1.58	7 (17%)	44,90,113	1.87	6 (13%)
15	CLA	A	1112	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	9 (19%)
15	CLA	A	1139	-	46,60,73	1.51	6 (13%)	51,97,113	2.06	12 (23%)
26	SF4	C	3003	7	0,12,12	0.00	-	-		
15	CLA	B	1201	-	42,56,73	1.59	9 (21%)	46,92,113	1.99	8 (17%)
15	CLA	1	603	-	36,53,73	1.78	9 (25%)	39,89,113	2.02	7 (17%)
15	CLA	B	1225	-	43,57,73	1.49	7 (16%)	46,93,113	2.07	9 (19%)
15	CLA	F	1302	-	43,57,73	1.49	8 (18%)	46,93,113	1.99	9 (19%)
15	CLA	A	1121	-	43,57,73	1.53	8 (18%)	46,93,113	2.06	8 (17%)
15	CLA	A	1135	-	43,57,73	1.52	8 (18%)	46,93,113	2.11	8 (17%)
15	CLA	A	1101	-	36,53,73	1.71	7 (19%)	39,89,113	2.15	9 (23%)
14	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.29	16 (28%)
15	CLA	1	608	-	40,54,73	1.60	7 (17%)	44,90,113	2.03	6 (13%)
16	CHL	2	610	-	44,58,74	0.89	2 (4%)	43,94,114	1.42	11 (25%)
15	CLA	3	608	-	42,56,73	1.56	9 (21%)	46,92,113	1.96	8 (17%)
16	CHL	3	604	-	41,55,74	0.96	2 (4%)	41,91,114	1.56	10 (24%)
15	CLA	A	1137	-	43,57,73	1.54	8 (18%)	46,93,113	2.11	10 (21%)
15	CLA	B	1238	-	44,58,73	1.53	7 (15%)	49,95,113	2.05	9 (18%)
17	LHG	A	5002	-	23,23,48	0.52	0	26,29,54	1.44	3 (11%)
15	CLA	B	1232	-	43,57,73	1.55	8 (18%)	46,93,113	2.07	8 (17%)
15	CLA	3	603	-	36,53,73	1.68	9 (25%)	39,89,113	2.43	12 (30%)
12	LUT	2	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.24	15 (29%)
23	GSH	B	5031	-	12,19,19	2.46	3 (25%)	15,24,24	1.65	2 (13%)
20	CAC	3	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	B	1208	-	43,57,73	1.56	7 (16%)	46,93,113	2.06	9 (19%)
15	CLA	3	606	-	36,53,73	1.66	7 (19%)	39,89,113	2.07	9 (23%)
15	CLA	A	1131	-	44,58,73	1.53	8 (18%)	49,95,113	2.06	9 (18%)
15	CLA	A	1125	-	43,57,73	1.52	7 (16%)	46,93,113	2.05	8 (17%)
15	CLA	A	1105	-	43,57,73	1.55	8 (18%)	46,93,113	2.11	9 (19%)
16	CHL	1	609	1	44,58,74	0.96	2 (4%)	43,94,114	1.44	11 (25%)
14	BCR	B	4005	-	41,41,41	1.87	4 (9%)	56,56,56	4.47	14 (25%)
12	LUT	3	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.13	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1237	-	43,57,73	1.54	8 (18%)	46,93,113	2.07	9 (19%)
15	CLA	3	611	-	40,54,73	1.57	6 (15%)	44,90,113	1.99	6 (13%)
13	XAT	1	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
15	CLA	1	607	17	40,54,73	1.59	8 (20%)	44,90,113	1.93	6 (13%)
15	CLA	B	1212	-	36,53,73	1.65	7 (19%)	39,89,113	2.04	9 (23%)
16	CHL	2	613	-	37,54,74	1.05	3 (8%)	36,90,114	1.55	11 (30%)
15	CLA	2	606	-	40,54,73	1.63	8 (20%)	44,90,113	2.04	7 (15%)
15	CLA	A	1102	15	36,53,73	1.66	8 (22%)	39,89,113	2.11	7 (17%)
24	CL0	A	1011	-	44,58,73	2.71	16 (36%)	49,95,113	2.53	15 (30%)
15	CLA	A	1103	-	49,63,73	1.43	8 (16%)	55,101,113	1.95	10 (18%)
15	CLA	1	605	-	42,56,73	1.53	7 (16%)	46,92,113	2.04	10 (21%)
14	BCR	A	4002	-	41,41,41	1.88	4 (9%)	56,56,56	4.42	18 (32%)
16	CHL	4	611	-	44,58,74	1.02	3 (6%)	43,94,114	1.43	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	604	4	3/3/16/25	11/18/116/135	-
15	CLA	A	1124	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1133	-	3/3/16/25	7/18/116/135	-
14	BCR	B	4001	-	-	14/29/63/63	0/2/2/2
15	CLA	2	608	-	3/3/16/25	9/18/116/135	-
13	XAT	3	502	-	1/1/12/26	14/31/93/93	0/4/4/4
15	CLA	2	601	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1218	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1119	-	3/3/16/25	11/18/116/135	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1127	-	3/3/16/25	11/18/116/135	-
15	CLA	A	1134	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1130	-	3/3/18/25	15/25/123/135	-
12	LUT	4	501	-	-	7/29/67/67	0/2/2/2
14	BCR	4	503	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1205	-	3/3/16/25	9/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1117	-	3/3/16/25	7/18/116/135	-
15	CLA	A	1013	-	3/3/20/25	20/37/135/135	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1123	-	3/3/16/25	9/17/115/135	-
15	CLA	3	612	-	3/3/18/25	10/25/123/135	-
19	SQD	1	811	-	-	6/34/54/69	0/1/1/1
15	CLA	1	601	-	3/3/16/25	13/18/116/135	-
16	CHL	3	604	-	3/3/16/26	6/17/115/137	-
15	CLA	B	1227	-	3/3/16/25	3/11/111/135	-
15	CLA	A	1108	-	3/3/16/25	10/15/113/135	-
15	CLA	B	1214	-	3/3/16/25	10/18/116/135	-
15	CLA	4	601	4	3/3/16/25	9/18/116/135	-
21	DGD	4	811	-	-	14/34/74/95	0/2/2/2
15	CLA	B	1229	-	3/3/20/25	17/37/135/135	-
15	CLA	B	1206	6	3/3/16/25	9/18/116/135	-
25	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
21	DGD	B	5002	-	-	9/27/67/95	0/2/2/2
15	CLA	B	1209	-	3/3/16/25	8/15/113/135	-
16	CHL	4	610	-	4/4/16/26	5/17/115/137	-
15	CLA	4	607	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1204	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1136	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1211	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1109	15	3/3/16/25	8/18/116/135	-
15	CLA	A	1113	-	3/3/16/25	6/11/111/135	-
14	BCR	J	4003	-	-	14/29/63/63	0/2/2/2
15	CLA	4	608	-	3/3/16/25	6/15/113/135	-
15	CLA	F	1301	-	3/3/16/25	10/16/114/135	-
23	GSH	4	831	-	-	3/18/24/24	-
15	CLA	2	602	-	3/3/16/25	7/18/116/135	-
16	CHL	4	613	-	4/4/16/26	7/20/118/137	-
26	SF4	A	3001	5,6	-	-	0/6/5/5
15	CLA	2	607	-	3/3/16/25	12/18/116/135	-
15	CLA	B	1230	-	3/3/16/25	8/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1111	-	3/3/16/25	7/18/116/135	-
15	CLA	3	613	-	3/3/16/25	10/15/113/135	-
15	CLA	1	604	1	3/3/16/25	7/18/116/135	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	2	604	-	3/3/16/25	11/18/116/135	-
18	LMG	2	803	-	-	3/7/27/70	0/1/1/1
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1138	-	3/3/20/25	20/37/135/135	-
15	CLA	A	1128	-	3/3/16/25	10/18/116/135	-
15	CLA	J	1302	-	3/3/16/25	12/18/116/135	-
15	CLA	B	1231	6	3/3/19/25	11/31/129/135	-
14	BCR	4	505	-	-	19/29/63/63	0/2/2/2
13	XAT	4	502	-	1/1/12/26	6/31/93/93	0/4/4/4
15	CLA	A	1118	-	3/3/16/25	14/18/116/135	-
15	CLA	4	615	-	3/3/18/25	12/25/123/135	-
15	CLA	A	1129	-	3/3/16/25	12/17/115/135	-
18	LMG	2	802	-	-	8/20/40/70	0/1/1/1
15	CLA	B	1215	-	3/3/16/25	9/18/116/135	-
15	CLA	4	605	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1224	-	3/3/16/25	11/18/116/135	-
15	CLA	A	1104	-	3/3/19/25	17/31/129/135	-
15	CLA	B	1202	-	3/3/16/25	11/18/116/135	-
15	CLA	2	612	-	3/3/16/25	14/18/116/135	-
12	LUT	2	501	-	-	6/29/67/67	0/2/2/2
15	CLA	A	1115	-	3/3/16/25	10/18/116/135	-
15	CLA	3	605	-	3/3/16/25	5/15/113/135	-
15	CLA	A	1114	-	3/3/16/25	6/15/113/135	-
15	CLA	B	1022	-	3/3/17/25	7/19/117/135	-
15	CLA	3	615	-	3/3/16/25	6/15/113/135	-
15	CLA	B	1203	-	3/3/16/25	8/18/116/135	-
14	BCR	1	505	-	-	12/29/63/63	0/2/2/2
15	CLA	1	613	-	3/3/16/25	4/11/111/135	-
12	LUT	1	501	-	-	8/29/67/67	0/2/2/2
15	CLA	B	1207	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1220	-	3/3/18/25	12/25/123/135	-
18	LMG	1	803	-	-	6/16/36/70	0/1/1/1
15	CLA	3	610	-	3/3/16/25	7/18/116/135	-
15	CLA	B	1236	-	3/3/16/25	10/18/116/135	-
14	BCR	1	503	-	-	16/29/63/63	0/2/2/2
17	LHG	B	5001	15	-	13/23/23/53	-
15	CLA	4	606	-	3/3/16/25	11/18/116/135	-
15	CLA	1	602	-	3/3/16/25	11/15/113/135	-
15	CLA	B	1226	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1239	-	3/3/20/25	17/37/135/135	-
15	CLA	B	1216	-	3/3/16/25	10/18/116/135	-
17	LHG	1	801	15	-	11/26/26/53	-
15	CLA	A	1012	-	3/3/19/25	11/31/129/135	-
15	CLA	A	1110	-	3/3/16/25	8/18/116/135	-
14	BCR	2	503	-	-	14/29/63/63	0/2/2/2
15	CLA	A	1132	-	3/3/16/25	12/18/116/135	-
16	CHL	2	609	2	3/3/16/26	7/20/118/137	-
15	CLA	A	1122	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1240	17	3/3/20/25	19/37/135/135	-
15	CLA	B	1217	-	3/3/16/25	11/15/113/135	-
21	DGD	2	811	-	-	13/36/76/95	0/2/2/2
22	LMT	2	821	-	-	1/8/48/61	0/2/2/2
15	CLA	4	602	-	3/3/16/25	5/18/116/135	-
15	CLA	1	606	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1021	-	3/3/20/25	17/37/135/135	-
14	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	4	612	-	3/3/16/25	11/18/116/135	-
15	CLA	1	611	-	3/3/16/25	12/18/116/135	-
21	DGD	J	5001	-	-	5/14/54/95	0/2/2/2
15	CLA	B	1235	-	3/3/19/25	20/31/129/135	-
25	PQN	A	2001	-	-	12/23/43/43	0/2/2/2
15	CLA	3	601	-	3/3/16/25	12/18/116/135	-
13	XAT	2	502	-	1/1/12/26	3/31/93/93	0/4/4/4
15	CLA	B	1223	-	3/3/17/25	7/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1107	5	3/3/16/25	4/18/116/135	-
15	CLA	A	1120	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1141	-	3/3/17/25	9/19/117/135	-
15	CLA	B	1228	-	3/3/19/25	9/31/129/135	-
18	LMG	1	802	-	-	8/31/51/70	0/1/1/1
16	CHL	1	610	-	3/3/16/26	5/17/115/137	-
15	CLA	2	605	-	3/3/20/25	15/37/135/135	-
15	CLA	B	1222	-	3/3/16/25	9/18/116/135	-
26	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	1	612	-	4/4/19/25	8/27/125/135	-
15	CLA	2	615	2	3/3/17/25	9/19/117/135	-
14	BCR	F	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1140	-	3/3/18/25	13/25/123/135	-
14	BCR	A	4005	-	-	8/29/63/63	0/2/2/2
15	CLA	4	603	-	3/3/16/25	4/18/116/135	-
17	LHG	2	801	-	-	10/23/23/53	-
15	CLA	B	1023	-	3/3/19/25	15/31/129/135	-
15	CLA	B	1210	-	3/3/16/25	12/18/116/135	-
15	CLA	1	615	-	3/3/20/25	20/37/135/135	-
14	BCR	A	4004	-	-	10/29/63/63	0/2/2/2
15	CLA	4	609	4	3/3/16/25	7/18/116/135	-
15	CLA	A	1116	-	3/3/16/25	8/18/116/135	-
14	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
14	BCR	A	4006	-	-	15/29/63/63	0/2/2/2
14	BCR	3	504	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1234	-	3/3/16/25	8/18/116/135	-
14	BCR	3	503	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1221	-	3/3/16/25	7/18/116/135	-
16	CHL	2	611	-	4/4/16/26	1/18/116/137	-
17	LHG	A	5001	-	-	14/18/18/53	-
15	CLA	B	1219	-	3/3/16/25	9/18/116/135	-
14	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1126	-	3/3/16/25	9/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	603	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1112	-	3/3/16/25	7/18/116/135	-
15	CLA	A	1139	-	3/3/17/25	6/22/120/135	-
26	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	B	1201	-	3/3/16/25	10/17/115/135	-
15	CLA	1	603	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1225	-	3/3/16/25	8/18/116/135	-
15	CLA	F	1302	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1121	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1135	-	3/3/16/25	11/18/116/135	-
15	CLA	A	1101	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1213	-	3/3/16/25	9/18/116/135	-
15	CLA	1	608	-	3/3/16/25	7/15/113/135	-
16	CHL	2	610	-	4/4/16/26	8/20/118/137	-
15	CLA	3	608	-	3/3/16/25	7/17/115/135	-
15	CLA	A	1106	-	3/3/20/25	15/37/135/135	-
15	CLA	A	1137	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1238	-	3/3/17/25	8/19/117/135	-
17	LHG	A	5002	-	-	18/28/28/53	-
15	CLA	B	1232	-	3/3/16/25	8/18/116/135	-
15	CLA	3	603	-	3/3/16/25	6/11/111/135	-
15	CLA	3	607	-	3/3/17/25	11/19/117/135	-
23	GSH	B	5031	-	-	7/18/24/24	-
15	CLA	B	1208	-	3/3/16/25	7/18/116/135	-
15	CLA	3	606	-	3/3/16/25	5/11/111/135	-
15	CLA	A	1131	-	3/3/17/25	10/19/117/135	-
15	CLA	A	1125	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1105	-	3/3/16/25	9/18/116/135	-
16	CHL	1	609	1	4/4/16/26	6/20/118/137	-
14	BCR	B	4005	-	-	16/29/63/63	0/2/2/2
12	LUT	3	501	-	-	4/29/67/67	0/2/2/2
15	CLA	B	1237	-	3/3/16/25	11/18/116/135	-
15	CLA	3	611	-	3/3/16/25	9/15/113/135	-
13	XAT	1	502	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	1	607	17	3/3/16/25	9/15/113/135	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
16	CHL	2	613	-	3/3/16/26	2/13/113/137	-
15	CLA	2	606	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1102	15	3/3/16/25	5/11/111/135	-
24	CL0	A	1011	-	3/3/17/25	13/19/117/135	-
15	CLA	A	1103	-	3/3/18/25	16/25/123/135	-
15	CLA	1	605	-	3/3/16/25	10/17/115/135	-
15	CLA	B	1212	-	3/3/16/25	6/11/111/135	-
16	CHL	4	611	-	3/3/16/26	5/20/118/137	-

All (1175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4005	BCR	C11-C12	19.10	1.83	1.34
14	A	4005	BCR	C11-C10	15.97	1.92	1.43
12	1	501	LUT	C24-C25	14.94	1.51	1.33
12	3	501	LUT	C24-C25	14.66	1.51	1.33
12	4	501	LUT	C24-C25	14.54	1.51	1.33
12	2	501	LUT	C24-C25	14.53	1.51	1.33
15	B	1207	CLA	CHB-C4A	9.35	1.42	1.34
24	A	1011	CL0	MG-NA	9.00	2.27	2.06
14	A	4005	BCR	C12-C13	7.94	1.63	1.45
14	B	4002	BCR	C10-C9	7.68	1.46	1.35
14	A	4002	BCR	C10-C9	7.58	1.45	1.35
14	4	505	BCR	C10-C9	7.55	1.45	1.35
14	B	4006	BCR	C10-C9	7.49	1.45	1.35
14	B	4003	BCR	C10-C9	7.46	1.45	1.35
14	A	4007	BCR	C10-C9	7.45	1.45	1.35
14	A	4004	BCR	C10-C9	7.42	1.45	1.35
14	3	503	BCR	C10-C9	7.37	1.45	1.35
14	2	503	BCR	C10-C9	7.35	1.45	1.35
14	1	503	BCR	C10-C9	7.33	1.45	1.35
14	1	505	BCR	C10-C9	7.32	1.45	1.35
14	B	4005	BCR	C10-C9	7.24	1.45	1.35
15	B	1229	CLA	MG-NA	7.23	2.23	2.06
14	3	504	BCR	C10-C9	7.23	1.45	1.35
14	A	4003	BCR	C10-C9	7.19	1.45	1.35
14	4	503	BCR	C10-C9	7.18	1.45	1.35
14	J	4003	BCR	C10-C9	7.15	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1215	CLA	MG-NA	7.12	2.23	2.06
14	F	4002	BCR	C10-C9	7.06	1.45	1.35
15	B	1223	CLA	MG-NA	7.03	2.23	2.06
14	B	4001	BCR	C10-C9	6.98	1.45	1.35
15	A	1126	CLA	MG-NA	6.93	2.22	2.06
15	B	1227	CLA	MG-NA	6.88	2.22	2.06
15	2	606	CLA	MG-NA	6.87	2.22	2.06
15	3	601	CLA	MG-NA	6.85	2.22	2.06
15	B	1021	CLA	MG-NA	6.85	2.22	2.06
15	B	1230	CLA	MG-NA	6.84	2.22	2.06
15	A	1108	CLA	MG-NA	6.84	2.22	2.06
15	1	603	CLA	MG-NA	6.82	2.22	2.06
14	J	4001	BCR	C10-C9	6.81	1.44	1.35
15	4	604	CLA	MG-NA	6.80	2.22	2.06
14	A	4006	BCR	C10-C9	6.80	1.44	1.35
15	3	615	CLA	MG-NA	6.78	2.22	2.06
15	4	605	CLA	MG-NA	6.74	2.22	2.06
14	J	4002	BCR	C10-C9	6.73	1.44	1.35
15	2	602	CLA	MG-NA	6.71	2.22	2.06
15	A	1101	CLA	MG-NA	6.70	2.22	2.06
15	1	611	CLA	MG-NA	6.67	2.22	2.06
15	2	607	CLA	MG-NA	6.65	2.22	2.06
15	B	1208	CLA	MG-NA	6.62	2.22	2.06
15	A	1115	CLA	MG-NA	6.61	2.22	2.06
15	A	1123	CLA	MG-NA	6.61	2.22	2.06
15	B	1222	CLA	MG-NA	6.60	2.22	2.06
14	B	4004	BCR	C10-C9	6.57	1.44	1.35
15	A	1106	CLA	MG-NA	6.57	2.21	2.06
15	B	1221	CLA	MG-NA	6.55	2.21	2.06
15	2	605	CLA	MG-NA	6.53	2.21	2.06
15	F	1301	CLA	MG-NA	6.52	2.21	2.06
15	4	612	CLA	MG-NA	6.52	2.21	2.06
15	B	1238	CLA	MG-NA	6.51	2.21	2.06
15	B	1239	CLA	MG-NA	6.50	2.21	2.06
15	B	1214	CLA	MG-NA	6.50	2.21	2.06
15	1	612	CLA	MG-NA	6.50	2.21	2.06
15	B	1204	CLA	MG-NA	6.49	2.21	2.06
15	B	1231	CLA	MG-NA	6.48	2.21	2.06
15	B	1234	CLA	MG-NA	6.48	2.21	2.06
15	A	1127	CLA	MG-NA	6.48	2.21	2.06
15	A	1129	CLA	MG-NA	6.47	2.21	2.06
15	B	1202	CLA	MG-NA	6.47	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	CLA	MG-NA	6.46	2.21	2.06
15	B	1232	CLA	MG-NA	6.46	2.21	2.06
15	3	607	CLA	MG-NA	6.45	2.21	2.06
15	B	1220	CLA	MG-NA	6.45	2.21	2.06
15	A	1141	CLA	MG-NA	6.45	2.21	2.06
15	B	1240	CLA	MG-NA	6.44	2.21	2.06
15	1	615	CLA	MG-NA	6.43	2.21	2.06
15	B	1201	CLA	MG-NA	6.43	2.21	2.06
15	A	1120	CLA	MG-NA	6.43	2.21	2.06
15	A	1107	CLA	MG-NA	6.43	2.21	2.06
15	4	606	CLA	MG-NA	6.42	2.21	2.06
15	A	1102	CLA	MG-NA	6.41	2.21	2.06
15	A	1128	CLA	MG-NA	6.41	2.21	2.06
15	A	1139	CLA	MG-NA	6.40	2.21	2.06
15	3	608	CLA	MG-NA	6.40	2.21	2.06
15	4	609	CLA	MG-NA	6.39	2.21	2.06
15	3	603	CLA	MG-NA	6.39	2.21	2.06
15	A	1112	CLA	MG-NA	6.38	2.21	2.06
15	B	1209	CLA	MG-NA	6.38	2.21	2.06
15	A	1136	CLA	MG-NA	6.38	2.21	2.06
15	A	1121	CLA	MG-NA	6.38	2.21	2.06
15	A	1130	CLA	MG-NA	6.37	2.21	2.06
15	4	615	CLA	MG-NA	6.37	2.21	2.06
15	A	1119	CLA	MG-NA	6.37	2.21	2.06
15	3	613	CLA	MG-NA	6.37	2.21	2.06
15	B	1206	CLA	MG-NA	6.37	2.21	2.06
15	3	611	CLA	MG-NA	6.37	2.21	2.06
15	3	606	CLA	MG-NA	6.37	2.21	2.06
15	A	1131	CLA	MG-NA	6.36	2.21	2.06
15	A	1125	CLA	MG-NA	6.36	2.21	2.06
15	2	612	CLA	MG-NA	6.36	2.21	2.06
15	A	1133	CLA	MG-NA	6.36	2.21	2.06
15	B	1212	CLA	MG-NA	6.36	2.21	2.06
15	A	1113	CLA	MG-NA	6.35	2.21	2.06
15	B	1205	CLA	MG-NA	6.35	2.21	2.06
15	A	1137	CLA	MG-NA	6.33	2.21	2.06
15	B	1023	CLA	MG-NA	6.33	2.21	2.06
15	A	1135	CLA	MG-NA	6.32	2.21	2.06
15	A	1109	CLA	MG-NA	6.32	2.21	2.06
15	A	1134	CLA	MG-NA	6.32	2.21	2.06
15	A	1105	CLA	MG-NA	6.31	2.21	2.06
15	B	1203	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	607	CLA	MG-NA	6.31	2.21	2.06
15	A	1012	CLA	MG-NA	6.31	2.21	2.06
15	A	1114	CLA	MG-NA	6.30	2.21	2.06
15	B	1225	CLA	MG-NA	6.30	2.21	2.06
15	B	1211	CLA	MG-NA	6.30	2.21	2.06
15	J	1302	CLA	MG-NA	6.30	2.21	2.06
15	1	604	CLA	MG-NA	6.30	2.21	2.06
15	A	1117	CLA	MG-NA	6.29	2.21	2.06
15	1	606	CLA	MG-NA	6.29	2.21	2.06
15	A	1103	CLA	MG-NA	6.28	2.21	2.06
15	A	1124	CLA	MG-NA	6.28	2.21	2.06
15	1	608	CLA	MG-NA	6.28	2.21	2.06
15	A	1104	CLA	MG-NA	6.27	2.21	2.06
15	A	1118	CLA	MG-NA	6.26	2.21	2.06
15	4	608	CLA	MG-NA	6.26	2.21	2.06
15	A	1138	CLA	MG-NA	6.25	2.21	2.06
15	B	1218	CLA	MG-NA	6.24	2.21	2.06
15	B	1217	CLA	MG-NA	6.24	2.21	2.06
15	1	602	CLA	MG-NA	6.24	2.21	2.06
15	A	1132	CLA	MG-NA	6.23	2.21	2.06
15	A	1122	CLA	MG-NA	6.23	2.21	2.06
15	2	608	CLA	MG-NA	6.22	2.21	2.06
14	4	503	BCR	C24-C23	6.22	1.51	1.33
15	A	1140	CLA	MG-NA	6.18	2.21	2.06
15	A	1013	CLA	MG-NA	6.18	2.21	2.06
15	3	610	CLA	MG-NA	6.18	2.21	2.06
15	B	1022	CLA	MG-NA	6.16	2.20	2.06
15	B	1228	CLA	MG-NA	6.13	2.20	2.06
15	4	603	CLA	MG-NA	6.12	2.20	2.06
15	A	1116	CLA	MG-NA	6.12	2.20	2.06
15	2	615	CLA	MG-NA	6.10	2.20	2.06
15	3	612	CLA	MG-NA	6.10	2.20	2.06
15	B	1224	CLA	MG-NA	6.07	2.20	2.06
15	B	1226	CLA	MG-NA	6.07	2.20	2.06
15	1	613	CLA	MG-NA	6.05	2.20	2.06
15	2	603	CLA	MG-NA	6.04	2.20	2.06
15	B	1236	CLA	MG-NA	6.02	2.20	2.06
15	1	601	CLA	MG-NA	6.02	2.20	2.06
15	A	1110	CLA	MG-NA	6.02	2.20	2.06
15	B	1235	CLA	MG-NA	6.02	2.20	2.06
15	4	602	CLA	MG-NA	6.01	2.20	2.06
15	2	604	CLA	MG-NA	5.97	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1219	CLA	MG-NA	5.94	2.20	2.06
15	B	1210	CLA	MG-NA	5.94	2.20	2.06
14	3	503	BCR	C24-C23	5.93	1.51	1.33
15	A	1111	CLA	MG-NA	5.92	2.20	2.06
15	1	605	CLA	MG-NA	5.90	2.20	2.06
15	4	601	CLA	MG-NA	5.89	2.20	2.06
14	B	4006	BCR	C24-C23	5.89	1.50	1.33
15	3	605	CLA	MG-NA	5.89	2.20	2.06
15	4	607	CLA	MG-NA	5.88	2.20	2.06
14	1	505	BCR	C24-C23	5.84	1.50	1.33
14	4	505	BCR	C24-C23	5.84	1.50	1.33
15	F	1302	CLA	MG-NA	5.83	2.20	2.06
14	2	503	BCR	C24-C23	5.82	1.50	1.33
14	F	4002	BCR	C24-C23	5.82	1.50	1.33
14	B	4001	BCR	C24-C23	5.80	1.50	1.33
14	A	4004	BCR	C24-C23	5.79	1.50	1.33
14	A	4002	BCR	C24-C23	5.78	1.50	1.33
14	A	4007	BCR	C24-C23	5.78	1.50	1.33
14	J	4002	BCR	C24-C23	5.78	1.50	1.33
14	A	4005	BCR	C24-C23	5.77	1.50	1.33
15	B	1216	CLA	MG-NA	5.76	2.20	2.06
14	B	4002	BCR	C24-C23	5.76	1.50	1.33
14	J	4001	BCR	C24-C23	5.76	1.50	1.33
14	3	504	BCR	C24-C23	5.72	1.50	1.33
14	B	4005	BCR	C24-C23	5.69	1.50	1.33
15	2	601	CLA	MG-NA	5.67	2.19	2.06
14	B	4003	BCR	C24-C23	5.64	1.50	1.33
23	B	5031	GSH	CD1-N2	5.61	1.46	1.34
14	B	4004	BCR	C24-C23	5.60	1.50	1.33
14	J	4003	BCR	C24-C23	5.58	1.49	1.33
15	B	1213	CLA	MG-NA	5.57	2.19	2.06
14	1	503	BCR	C24-C23	5.56	1.49	1.33
14	A	4003	BCR	C24-C23	5.56	1.49	1.33
23	4	831	GSH	C2-N3	5.52	1.45	1.33
23	B	5031	GSH	C2-N3	5.50	1.45	1.33
23	4	831	GSH	CD1-N2	5.41	1.45	1.34
14	A	4006	BCR	C24-C23	5.31	1.49	1.33
14	J	4001	BCR	C11-C12	-5.28	1.21	1.34
14	2	503	BCR	C11-C12	-5.20	1.21	1.34
14	1	505	BCR	C11-C12	-5.16	1.21	1.34
15	B	1207	CLA	C3B-C4B	5.15	1.49	1.39
14	A	4006	BCR	C11-C12	-5.13	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1011	CL0	O2D-CGD	5.12	1.45	1.33
14	J	4003	BCR	C11-C12	-5.11	1.21	1.34
24	A	1011	CL0	CHC-C1C	5.10	1.48	1.35
14	3	504	BCR	C11-C12	-5.09	1.21	1.34
14	B	4004	BCR	C11-C12	-5.09	1.21	1.34
14	4	503	BCR	C11-C12	-5.09	1.21	1.34
14	B	4001	BCR	C11-C12	-5.08	1.21	1.34
14	1	503	BCR	C11-C12	-5.07	1.21	1.34
14	B	4002	BCR	C11-C12	-5.05	1.21	1.34
15	B	1207	CLA	C3A-C2A	-5.05	1.39	1.52
14	A	4002	BCR	C11-C12	-5.05	1.21	1.34
14	A	4007	BCR	C11-C12	-5.04	1.21	1.34
14	B	4005	BCR	C11-C12	-5.03	1.21	1.34
24	A	1011	CL0	O2A-C1	5.01	1.60	1.46
14	B	4003	BCR	C11-C12	-5.00	1.21	1.34
14	A	4004	BCR	C11-C12	-4.99	1.21	1.34
14	F	4002	BCR	C11-C12	-4.99	1.21	1.34
14	3	503	BCR	C11-C12	-4.99	1.21	1.34
24	A	1011	CL0	C3C-C2C	4.92	1.47	1.36
14	A	4003	BCR	C11-C12	-4.89	1.22	1.34
14	J	4002	BCR	C11-C12	-4.89	1.22	1.34
14	4	505	BCR	C11-C12	-4.81	1.22	1.34
24	A	1011	CL0	OBD-CAD	4.80	1.29	1.22
14	B	4006	BCR	C11-C12	-4.77	1.22	1.34
14	B	4005	BCR	C16-C17	-4.57	1.29	1.43
21	2	811	DGD	O1G-C1A	4.43	1.46	1.33
14	J	4001	BCR	C16-C17	-4.41	1.29	1.43
14	A	4006	BCR	C16-C17	-4.40	1.29	1.43
14	1	503	BCR	C16-C17	-4.37	1.29	1.43
14	4	503	BCR	C16-C17	-4.37	1.29	1.43
21	4	811	DGD	O1G-C1A	4.35	1.46	1.33
14	J	4002	BCR	C16-C17	-4.34	1.30	1.43
14	3	504	BCR	C16-C17	-4.33	1.30	1.43
21	B	5002	DGD	O1G-C1A	4.32	1.46	1.33
14	A	4004	BCR	C16-C17	-4.30	1.30	1.43
14	B	4004	BCR	C16-C17	-4.28	1.30	1.43
14	J	4003	BCR	C16-C17	-4.21	1.30	1.43
14	3	503	BCR	C16-C17	-4.20	1.30	1.43
14	B	4002	BCR	C16-C17	-4.19	1.30	1.43
24	A	1011	CL0	C3D-C2D	4.19	1.46	1.39
14	A	4002	BCR	C16-C17	-4.19	1.30	1.43
14	A	4005	BCR	C16-C17	-4.19	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	503	BCR	C16-C17	-4.18	1.30	1.43
14	A	4003	BCR	C16-C17	-4.18	1.30	1.43
14	A	4007	BCR	C16-C17	-4.18	1.30	1.43
14	F	4002	BCR	C16-C17	-4.16	1.30	1.43
24	A	1011	CL0	C3B-C2B	4.15	1.46	1.40
14	B	4001	BCR	C16-C17	-4.13	1.30	1.43
14	4	505	BCR	C16-C17	-4.11	1.30	1.43
14	1	505	BCR	C16-C17	-4.08	1.30	1.43
14	B	4003	BCR	C16-C17	-4.01	1.31	1.43
24	A	1011	CL0	MG-NC	3.95	2.15	2.06
16	1	610	CHL	C4B-NB	3.94	1.38	1.35
14	B	4006	BCR	C16-C17	-3.86	1.31	1.43
15	A	1012	CLA	C1C-NC	-3.81	1.32	1.37
15	B	1207	CLA	C1B-NB	3.71	1.38	1.35
15	A	1127	CLA	C1C-NC	-3.68	1.32	1.37
15	B	1207	CLA	C2B-C1B	3.68	1.46	1.39
15	4	612	CLA	C1C-NC	-3.64	1.32	1.37
15	4	605	CLA	C1C-NC	-3.59	1.32	1.37
16	2	611	CHL	C4B-NB	3.57	1.38	1.35
15	B	1227	CLA	C1C-NC	-3.54	1.32	1.37
15	B	1218	CLA	C1C-NC	-3.53	1.32	1.37
15	B	1229	CLA	C1C-NC	-3.53	1.32	1.37
15	A	1013	CLA	C1C-NC	-3.50	1.32	1.37
15	1	604	CLA	C1C-NC	-3.50	1.32	1.37
15	1	613	CLA	CBB-CAB	3.50	1.52	1.29
15	1	612	CLA	C1C-NC	-3.48	1.32	1.37
15	1	603	CLA	C1C-NC	-3.48	1.32	1.37
16	2	609	CHL	C4B-NB	3.47	1.38	1.35
15	J	1302	CLA	C1C-NC	-3.47	1.32	1.37
15	4	606	CLA	CBB-CAB	3.46	1.52	1.29
15	B	1218	CLA	CBB-CAB	3.46	1.52	1.29
15	4	607	CLA	CBB-CAB	3.46	1.52	1.29
15	4	605	CLA	CBB-CAB	3.46	1.52	1.29
15	4	615	CLA	CBB-CAB	3.45	1.52	1.29
15	F	1302	CLA	CBB-CAB	3.44	1.52	1.29
24	A	1011	CL0	C1D-C2D	3.43	1.50	1.42
15	3	613	CLA	C1B-NB	3.42	1.38	1.35
15	B	1208	CLA	CBB-CAB	3.41	1.51	1.29
15	1	615	CLA	CBB-CAB	3.40	1.51	1.29
15	B	1228	CLA	CBB-CAB	3.40	1.51	1.29
15	B	1216	CLA	CBB-CAB	3.39	1.51	1.29
15	B	1222	CLA	C1C-NC	-3.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1231	CLA	CBB-CAB	3.39	1.51	1.29
15	A	1131	CLA	C1C-NC	-3.39	1.32	1.37
15	A	1135	CLA	CBB-CAB	3.39	1.51	1.29
16	4	610	CHL	CBB-CAB	3.39	1.51	1.29
15	B	1213	CLA	CBB-CAB	3.39	1.51	1.29
15	A	1138	CLA	CBB-CAB	3.39	1.51	1.29
15	A	1127	CLA	CBB-CAB	3.39	1.51	1.29
15	B	1201	CLA	CBB-CAB	3.39	1.51	1.29
15	B	1206	CLA	CBB-CAB	3.39	1.51	1.29
15	B	1201	CLA	C1C-NC	-3.39	1.32	1.37
15	2	608	CLA	CBB-CAB	3.38	1.51	1.29
15	A	1111	CLA	CBB-CAB	3.38	1.51	1.29
15	A	1133	CLA	CBB-CAB	3.38	1.51	1.29
15	4	604	CLA	CBB-CAB	3.38	1.51	1.29
15	B	1212	CLA	CBB-CAB	3.38	1.51	1.29
15	4	602	CLA	CBB-CAB	3.38	1.51	1.29
15	B	1215	CLA	C1C-NC	-3.38	1.32	1.37
15	1	605	CLA	CBB-CAB	3.38	1.51	1.29
15	B	1229	CLA	CBB-CAB	3.37	1.51	1.29
16	2	610	CHL	CBB-CAB	3.37	1.51	1.29
15	3	601	CLA	CBB-CAB	3.37	1.51	1.29
15	B	1223	CLA	CBB-CAB	3.37	1.51	1.29
15	B	1237	CLA	CBB-CAB	3.37	1.51	1.29
15	3	603	CLA	CBB-CAB	3.37	1.51	1.29
15	2	612	CLA	CBB-CAB	3.37	1.51	1.29
15	2	603	CLA	CBB-CAB	3.37	1.51	1.29
15	A	1140	CLA	CBB-CAB	3.37	1.51	1.29
15	B	1204	CLA	CBB-CAB	3.36	1.51	1.29
15	1	606	CLA	CBB-CAB	3.36	1.51	1.29
16	4	611	CHL	C4B-NB	3.36	1.38	1.35
15	A	1122	CLA	CBB-CAB	3.36	1.51	1.29
15	B	1236	CLA	CBB-CAB	3.36	1.51	1.29
15	A	1139	CLA	CBB-CAB	3.36	1.51	1.29
15	A	1116	CLA	CBB-CAB	3.36	1.51	1.29
15	A	1131	CLA	CBB-CAB	3.36	1.51	1.29
15	A	1119	CLA	CBB-CAB	3.36	1.51	1.29
15	B	1023	CLA	CBB-CAB	3.36	1.51	1.29
15	A	1128	CLA	CBB-CAB	3.36	1.51	1.29
15	3	605	CLA	C1C-NC	-3.36	1.32	1.37
15	A	1110	CLA	CBB-CAB	3.36	1.51	1.29
15	B	1225	CLA	CBB-CAB	3.36	1.51	1.29
15	B	1226	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	1301	CLA	CBB-CAB	3.36	1.51	1.29
15	B	1205	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1129	CLA	CBB-CAB	3.35	1.51	1.29
15	B	1203	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1141	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1121	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1137	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1117	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1115	CLA	CBB-CAB	3.35	1.51	1.29
15	A	1140	CLA	C1C-NC	-3.35	1.32	1.37
15	3	605	CLA	CBB-CAB	3.35	1.51	1.29
15	B	1239	CLA	CBB-CAB	3.35	1.51	1.29
16	3	604	CHL	CBB-CAB	3.35	1.51	1.29
16	4	613	CHL	C4B-NB	3.35	1.38	1.35
15	B	1215	CLA	CBB-CAB	3.35	1.51	1.29
15	1	601	CLA	CBB-CAB	3.35	1.51	1.29
15	B	1221	CLA	CBB-CAB	3.34	1.51	1.29
15	4	601	CLA	CBB-CAB	3.34	1.51	1.29
15	A	1128	CLA	C1C-NC	-3.34	1.32	1.37
15	A	1130	CLA	CBB-CAB	3.34	1.51	1.29
15	4	612	CLA	CBB-CAB	3.34	1.51	1.29
15	1	602	CLA	C1C-NC	-3.34	1.32	1.37
15	A	1114	CLA	CBB-CAB	3.34	1.51	1.29
15	B	1209	CLA	CBB-CAB	3.34	1.51	1.29
15	3	613	CLA	CBB-CAB	3.34	1.51	1.29
15	A	1013	CLA	CBB-CAB	3.34	1.51	1.29
15	4	608	CLA	CBB-CAB	3.34	1.51	1.29
15	2	612	CLA	C1C-NC	-3.34	1.32	1.37
15	A	1118	CLA	CBB-CAB	3.34	1.51	1.29
15	1	602	CLA	CBB-CAB	3.34	1.51	1.29
15	2	607	CLA	CBB-CAB	3.34	1.51	1.29
15	A	1132	CLA	CBB-CAB	3.34	1.51	1.29
15	3	606	CLA	CBB-CAB	3.34	1.51	1.29
15	1	608	CLA	CBB-CAB	3.33	1.51	1.29
15	3	610	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1120	CLA	CBB-CAB	3.33	1.51	1.29
15	3	607	CLA	CBB-CAB	3.33	1.51	1.29
15	B	1204	CLA	C1C-NC	-3.33	1.32	1.37
15	B	1210	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1102	CLA	CBB-CAB	3.33	1.51	1.29
15	4	609	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1105	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1021	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1103	CLA	CBB-CAB	3.33	1.51	1.29
15	B	1220	CLA	CBB-CAB	3.33	1.51	1.29
15	2	605	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1107	CLA	CBB-CAB	3.33	1.51	1.29
15	A	1130	CLA	C1C-NC	-3.33	1.32	1.37
15	A	1134	CLA	CBB-CAB	3.33	1.51	1.29
16	2	609	CHL	CBB-CAB	3.32	1.51	1.29
15	2	602	CLA	CBB-CAB	3.32	1.51	1.29
16	1	610	CHL	CBB-CAB	3.32	1.51	1.29
15	1	607	CLA	CBB-CAB	3.32	1.51	1.29
15	B	1217	CLA	CBB-CAB	3.32	1.51	1.29
15	A	1138	CLA	C1C-NC	-3.32	1.32	1.37
15	2	606	CLA	CBB-CAB	3.32	1.51	1.29
15	B	1222	CLA	CBB-CAB	3.32	1.51	1.29
15	A	1113	CLA	CBB-CAB	3.32	1.51	1.29
15	3	608	CLA	CBB-CAB	3.32	1.51	1.29
15	1	604	CLA	CBB-CAB	3.32	1.51	1.29
15	B	1227	CLA	CBB-CAB	3.32	1.51	1.29
15	4	602	CLA	C1C-NC	-3.32	1.32	1.37
15	B	1234	CLA	CBB-CAB	3.31	1.51	1.29
15	A	1123	CLA	CBB-CAB	3.31	1.51	1.29
15	A	1126	CLA	CBB-CAB	3.31	1.51	1.29
15	4	601	CLA	C1C-NC	-3.31	1.32	1.37
15	1	603	CLA	CBB-CAB	3.31	1.51	1.29
15	A	1104	CLA	CBB-CAB	3.31	1.51	1.29
15	2	615	CLA	CBB-CAB	3.31	1.51	1.29
15	1	612	CLA	CBB-CAB	3.31	1.51	1.29
15	A	1133	CLA	C1C-NC	-3.31	1.32	1.37
15	B	1202	CLA	CBB-CAB	3.31	1.51	1.29
15	A	1124	CLA	CBB-CAB	3.31	1.51	1.29
15	4	606	CLA	C1C-NC	-3.31	1.32	1.37
15	2	601	CLA	CBB-CAB	3.31	1.51	1.29
15	B	1214	CLA	CBB-CAB	3.30	1.51	1.29
15	1	611	CLA	CBB-CAB	3.30	1.51	1.29
15	2	601	CLA	C1C-NC	-3.30	1.32	1.37
15	B	1238	CLA	CBB-CAB	3.30	1.51	1.29
16	2	613	CHL	CBB-CAB	3.30	1.51	1.29
15	A	1106	CLA	CBB-CAB	3.30	1.51	1.29
15	3	606	CLA	C1C-NC	-3.30	1.32	1.37
15	A	1109	CLA	CBB-CAB	3.30	1.51	1.29
15	3	615	CLA	CBB-CAB	3.30	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1136	CLA	CBB-CAB	3.29	1.51	1.29
15	B	1224	CLA	CBB-CAB	3.29	1.51	1.29
15	A	1108	CLA	CBB-CAB	3.29	1.51	1.29
15	B	1232	CLA	CBB-CAB	3.29	1.51	1.29
15	A	1112	CLA	CBB-CAB	3.29	1.51	1.29
15	A	1012	CLA	CBB-CAB	3.29	1.51	1.29
16	1	609	CHL	CBB-CAB	3.29	1.51	1.29
15	A	1125	CLA	CBB-CAB	3.28	1.51	1.29
15	A	1101	CLA	CBB-CAB	3.28	1.51	1.29
16	2	611	CHL	CBB-CAB	3.28	1.51	1.29
15	3	612	CLA	CBB-CAB	3.28	1.51	1.29
15	4	609	CLA	C1C-NC	-3.27	1.32	1.37
15	1	601	CLA	C1C-NC	-3.27	1.32	1.37
15	B	1209	CLA	C1C-NC	-3.27	1.32	1.37
15	3	611	CLA	CBB-CAB	3.27	1.51	1.29
15	B	1217	CLA	C1C-NC	-3.26	1.32	1.37
15	B	1226	CLA	C1C-NC	-3.26	1.32	1.37
15	2	604	CLA	CBB-CAB	3.25	1.50	1.29
15	A	1139	CLA	C1C-NC	-3.25	1.33	1.37
16	4	611	CHL	CBB-CAB	3.24	1.50	1.29
16	4	613	CHL	CBB-CAB	3.24	1.50	1.29
15	B	1211	CLA	CBB-CAB	3.24	1.50	1.29
15	B	1223	CLA	C1C-NC	-3.24	1.33	1.37
15	A	1118	CLA	C1C-NC	-3.23	1.33	1.37
15	4	607	CLA	C1B-NB	3.23	1.38	1.35
15	A	1117	CLA	C1C-NC	-3.23	1.33	1.37
15	A	1108	CLA	C1C-NC	-3.23	1.33	1.37
15	2	607	CLA	C1C-NC	-3.23	1.33	1.37
15	1	611	CLA	C1C-NC	-3.23	1.33	1.37
15	B	1230	CLA	CBB-CAB	3.23	1.50	1.29
16	1	609	CHL	C4B-NB	3.22	1.38	1.35
15	4	603	CLA	CBB-CAB	3.22	1.50	1.29
15	A	1136	CLA	C1C-NC	-3.22	1.33	1.37
15	J	1302	CLA	CBB-CAB	3.22	1.50	1.29
15	3	603	CLA	C1C-NC	-3.22	1.33	1.37
15	A	1116	CLA	C1C-NC	-3.22	1.33	1.37
15	1	607	CLA	C1C-NC	-3.22	1.33	1.37
15	3	615	CLA	C1C-NC	-3.22	1.33	1.37
15	B	1240	CLA	C1C-NC	-3.21	1.33	1.37
15	B	1022	CLA	CBB-CAB	3.21	1.50	1.29
15	A	1112	CLA	C1C-NC	-3.21	1.33	1.37
15	B	1219	CLA	CBB-CAB	3.21	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1114	CLA	C1C-NC	-3.21	1.33	1.37
15	2	603	CLA	C1C-NC	-3.20	1.33	1.37
15	A	1132	CLA	C1C-NC	-3.20	1.33	1.37
15	A	1107	CLA	C1C-NC	-3.19	1.33	1.37
15	1	608	CLA	C1C-NC	-3.19	1.33	1.37
15	3	613	CLA	C1C-NC	-3.19	1.33	1.37
15	B	1240	CLA	CBB-CAB	3.19	1.50	1.29
15	1	606	CLA	C1C-NC	-3.19	1.33	1.37
15	3	608	CLA	C1C-NC	-3.19	1.33	1.37
15	B	1202	CLA	C1C-NC	-3.18	1.33	1.37
15	A	1101	CLA	C1C-NC	-3.17	1.33	1.37
15	4	608	CLA	C1C-NC	-3.17	1.33	1.37
15	B	1224	CLA	C1C-NC	-3.17	1.33	1.37
15	B	1207	CLA	MG-NA	-3.16	1.98	2.06
15	A	1119	CLA	C1C-NC	-3.16	1.33	1.37
15	B	1212	CLA	C1C-NC	-3.16	1.33	1.37
15	2	608	CLA	C1C-NC	-3.16	1.33	1.37
15	B	1021	CLA	C1C-NC	-3.15	1.33	1.37
15	B	1023	CLA	CHC-C1C	3.15	1.43	1.35
15	B	1211	CLA	C1C-NC	-3.13	1.33	1.37
15	B	1237	CLA	C1C-NC	-3.13	1.33	1.37
15	A	1109	CLA	C1C-NC	-3.13	1.33	1.37
15	A	1135	CLA	C1C-NC	-3.12	1.33	1.37
15	A	1115	CLA	C1C-NC	-3.12	1.33	1.37
15	B	1219	CLA	C1C-NC	-3.11	1.33	1.37
15	4	615	CLA	C1C-NC	-3.11	1.33	1.37
15	B	1208	CLA	C1C-NC	-3.11	1.33	1.37
16	2	613	CHL	C4B-NB	3.11	1.38	1.35
15	A	1129	CLA	C1C-NC	-3.11	1.33	1.37
15	B	1230	CLA	C1C-NC	-3.10	1.33	1.37
15	4	603	CLA	C1C-NC	-3.10	1.33	1.37
15	3	610	CLA	C1C-NC	-3.10	1.33	1.37
15	B	1235	CLA	CBB-CAB	3.10	1.49	1.29
15	A	1121	CLA	C1C-NC	-3.10	1.33	1.37
15	A	1102	CLA	C1C-NC	-3.10	1.33	1.37
15	A	1110	CLA	C1C-NC	-3.09	1.33	1.37
24	A	1011	CL0	C4B-CHC	3.09	1.49	1.41
15	B	1214	CLA	C1C-NC	-3.09	1.33	1.37
15	B	1216	CLA	C1C-NC	-3.08	1.33	1.37
15	3	612	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1141	CLA	C1C-NC	-3.08	1.33	1.37
15	B	1022	CLA	C1C-NC	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1220	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1111	CLA	C1C-NC	-3.08	1.33	1.37
18	1	802	LMG	C37-C36	-3.08	1.34	1.51
15	B	1221	CLA	C1C-NC	-3.08	1.33	1.37
15	B	1207	CLA	C3D-C2D	3.07	1.54	1.39
15	A	1105	CLA	C1C-NC	-3.07	1.33	1.37
15	2	615	CLA	C1C-NC	-3.07	1.33	1.37
15	B	1206	CLA	C1C-NC	-3.07	1.33	1.37
15	A	1113	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1103	CLA	C1C-NC	-3.06	1.33	1.37
15	B	1239	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1106	CLA	C1C-NC	-3.06	1.33	1.37
15	A	1137	CLA	C1C-NC	-3.05	1.33	1.37
15	F	1301	CLA	C1C-NC	-3.05	1.33	1.37
15	B	1232	CLA	C1C-NC	-3.05	1.33	1.37
15	B	1203	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1123	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1126	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1134	CLA	C1C-NC	-3.05	1.33	1.37
15	2	602	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1238	CLA	C1C-NC	-3.04	1.33	1.37
15	A	1122	CLA	C1C-NC	-3.02	1.33	1.37
15	3	607	CLA	C1C-NC	-3.02	1.33	1.37
15	3	611	CLA	C1C-NC	-3.01	1.33	1.37
15	4	607	CLA	C1C-NC	-3.01	1.33	1.37
15	B	1220	CLA	C3B-C2B	-3.01	1.36	1.40
16	3	604	CHL	C4B-NB	2.99	1.37	1.35
15	B	1205	CLA	C1C-NC	-2.98	1.33	1.37
15	A	1120	CLA	C1C-NC	-2.98	1.33	1.37
15	4	605	CLA	C3B-C2B	-2.97	1.36	1.40
15	B	1210	CLA	C1C-NC	-2.96	1.33	1.37
15	1	613	CLA	C1C-NC	-2.96	1.33	1.37
15	1	605	CLA	C1C-NC	-2.95	1.33	1.37
15	F	1301	CLA	CHC-C1C	2.94	1.42	1.35
15	3	601	CLA	C1C-NC	-2.94	1.33	1.37
15	2	604	CLA	C1C-NC	-2.93	1.33	1.37
15	A	1125	CLA	C1C-NC	-2.93	1.33	1.37
15	A	1140	CLA	C1B-NB	2.93	1.37	1.35
15	A	1012	CLA	C3B-C2B	-2.90	1.36	1.40
15	B	1231	CLA	CHC-C1C	2.90	1.42	1.35
15	B	1234	CLA	C1C-NC	-2.90	1.33	1.37
24	A	1011	CL0	C4C-C3C	2.89	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	615	CLA	C1C-NC	-2.89	1.33	1.37
15	A	1104	CLA	C1C-NC	-2.89	1.33	1.37
15	A	1101	CLA	CHC-C1C	2.88	1.42	1.35
15	B	1226	CLA	C1B-NB	2.87	1.37	1.35
15	A	1105	CLA	C3B-C2B	-2.84	1.36	1.40
15	2	605	CLA	C1C-NC	-2.84	1.33	1.37
15	F	1302	CLA	C1C-NC	-2.84	1.33	1.37
15	A	1126	CLA	CHC-C1C	2.83	1.42	1.35
15	4	604	CLA	CHC-C1C	2.83	1.42	1.35
15	B	1225	CLA	C1C-NC	-2.82	1.33	1.37
15	B	1214	CLA	CHC-C1C	2.82	1.42	1.35
15	2	608	CLA	CHC-C1C	2.82	1.42	1.35
15	A	1123	CLA	CHC-C1C	2.81	1.42	1.35
15	B	1219	CLA	CHC-C1C	2.81	1.42	1.35
15	B	1203	CLA	CHC-C1C	2.80	1.42	1.35
15	B	1210	CLA	CHC-C1C	2.80	1.42	1.35
15	4	607	CLA	CHC-C1C	2.80	1.42	1.35
15	4	605	CLA	CHC-C1C	2.80	1.42	1.35
15	B	1231	CLA	C1B-NB	2.79	1.37	1.35
15	B	1213	CLA	C1C-NC	-2.78	1.33	1.37
15	B	1022	CLA	CHC-C1C	2.78	1.42	1.35
15	B	1218	CLA	CHC-C1C	2.77	1.42	1.35
15	4	609	CLA	CHC-C1C	2.77	1.42	1.35
15	B	1205	CLA	CHC-C1C	2.77	1.42	1.35
15	3	601	CLA	CHC-C1C	2.77	1.42	1.35
15	A	1111	CLA	CHC-C1C	2.77	1.42	1.35
15	3	605	CLA	CHC-C1C	2.76	1.42	1.35
15	1	613	CLA	CHC-C1C	2.76	1.42	1.35
15	B	1238	CLA	CHC-C1C	2.75	1.42	1.35
15	A	1110	CLA	CHC-C1C	2.75	1.42	1.35
15	B	1223	CLA	C3B-C2B	-2.75	1.36	1.40
24	A	1011	CL0	CHD-C4C	2.75	1.49	1.41
15	A	1119	CLA	CHC-C1C	2.75	1.42	1.35
15	3	608	CLA	CHC-C1C	2.75	1.42	1.35
15	A	1013	CLA	C3B-C2B	-2.74	1.36	1.40
15	1	611	CLA	C3B-C2B	-2.74	1.36	1.40
15	B	1224	CLA	C1B-NB	2.74	1.37	1.35
15	2	606	CLA	C1C-NC	-2.74	1.33	1.37
15	A	1122	CLA	CHC-C1C	2.74	1.42	1.35
15	B	1206	CLA	CHC-C1C	2.74	1.42	1.35
15	B	1234	CLA	CHC-C1C	2.74	1.42	1.35
15	A	1137	CLA	CHC-C1C	2.74	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	601	CLA	CHC-C1C	2.73	1.42	1.35
16	2	613	CHL	C3B-C2B	-2.73	1.36	1.40
15	B	1201	CLA	CHC-C1C	2.73	1.42	1.35
15	A	1120	CLA	CHC-C1C	2.73	1.42	1.35
15	B	1231	CLA	C1C-NC	-2.72	1.33	1.37
15	2	602	CLA	CHC-C1C	2.72	1.41	1.35
15	B	1021	CLA	CHC-C1C	2.72	1.41	1.35
15	A	1111	CLA	MG-NC	2.72	2.12	2.06
15	A	1113	CLA	CHC-C1C	2.72	1.41	1.35
15	B	1232	CLA	C1B-NB	2.72	1.37	1.35
15	4	612	CLA	CHC-C1C	2.71	1.41	1.35
15	B	1022	CLA	C1B-NB	2.71	1.37	1.35
15	A	1108	CLA	CHC-C1C	2.71	1.41	1.35
15	A	1012	CLA	CHC-C1C	2.70	1.41	1.35
15	1	608	CLA	CHC-C1C	2.70	1.41	1.35
15	B	1223	CLA	CHC-C1C	2.70	1.41	1.35
15	F	1302	CLA	CHC-C1C	2.70	1.41	1.35
15	A	1125	CLA	CHC-C1C	2.69	1.41	1.35
15	1	606	CLA	CHC-C1C	2.69	1.41	1.35
15	F	1301	CLA	C3B-C2B	-2.69	1.36	1.40
15	B	1239	CLA	CHC-C1C	2.69	1.41	1.35
15	B	1208	CLA	C1B-NB	2.69	1.37	1.35
15	A	1117	CLA	C3B-C2B	-2.69	1.36	1.40
15	A	1128	CLA	CHC-C1C	2.69	1.41	1.35
15	B	1212	CLA	CHC-C1C	2.69	1.41	1.35
15	1	602	CLA	CHC-C1C	2.68	1.41	1.35
15	B	1237	CLA	CHC-C1C	2.68	1.41	1.35
15	A	1115	CLA	CHC-C1C	2.68	1.41	1.35
15	B	1228	CLA	CHC-C1C	2.68	1.41	1.35
15	B	1225	CLA	CHC-C1C	2.68	1.41	1.35
15	1	605	CLA	C1B-NB	2.68	1.37	1.35
15	1	607	CLA	C1B-NB	2.68	1.37	1.35
15	1	612	CLA	CHC-C1C	2.68	1.41	1.35
15	3	606	CLA	CHC-C1C	2.67	1.41	1.35
15	A	1109	CLA	CHC-C1C	2.67	1.41	1.35
15	A	1121	CLA	CHC-C1C	2.67	1.41	1.35
15	1	604	CLA	CHC-C1C	2.67	1.41	1.35
15	A	1134	CLA	CHC-C1C	2.67	1.41	1.35
15	B	1224	CLA	CHC-C1C	2.67	1.41	1.35
15	A	1138	CLA	CHC-C1C	2.67	1.41	1.35
15	3	607	CLA	CHC-C1C	2.67	1.41	1.35
15	B	1220	CLA	CHC-C1C	2.67	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	608	CLA	C3B-C2B	-2.67	1.36	1.40
15	B	1217	CLA	CHC-C1C	2.67	1.41	1.35
15	B	1211	CLA	C1B-NB	2.66	1.37	1.35
15	2	607	CLA	CHC-C1C	2.66	1.41	1.35
15	1	601	CLA	CHC-C1C	2.66	1.41	1.35
15	1	607	CLA	CHC-C1C	2.66	1.41	1.35
15	B	1204	CLA	CHC-C1C	2.66	1.41	1.35
15	A	1133	CLA	CHC-C1C	2.66	1.41	1.35
15	A	1130	CLA	CHC-C1C	2.66	1.41	1.35
15	A	1124	CLA	CHC-C1C	2.66	1.41	1.35
15	B	1226	CLA	CHC-C1C	2.66	1.41	1.35
15	A	1133	CLA	C1B-NB	2.66	1.37	1.35
15	2	615	CLA	CHC-C1C	2.65	1.41	1.35
15	2	606	CLA	CHC-C1C	2.65	1.41	1.35
15	4	601	CLA	CHC-C1C	2.65	1.41	1.35
15	A	1141	CLA	CHC-C1C	2.65	1.41	1.35
15	A	1104	CLA	CHC-C1C	2.65	1.41	1.35
15	3	613	CLA	CHC-C1C	2.65	1.41	1.35
15	A	1135	CLA	CHC-C1C	2.65	1.41	1.35
15	4	602	CLA	CHC-C1C	2.65	1.41	1.35
15	A	1117	CLA	CHC-C1C	2.65	1.41	1.35
15	1	603	CLA	CHC-C1C	2.65	1.41	1.35
15	A	1118	CLA	CHC-C1C	2.64	1.41	1.35
15	B	1209	CLA	CHC-C1C	2.64	1.41	1.35
15	3	612	CLA	CHC-C1C	2.64	1.41	1.35
15	2	605	CLA	CHC-C1C	2.64	1.41	1.35
15	A	1139	CLA	CHC-C1C	2.64	1.41	1.35
15	B	1227	CLA	C3B-C2B	-2.64	1.36	1.40
15	A	1124	CLA	C1C-NC	-2.64	1.33	1.37
15	B	1229	CLA	CHC-C1C	2.63	1.41	1.35
15	B	1232	CLA	CHC-C1C	2.63	1.41	1.35
15	A	1116	CLA	CHC-C1C	2.62	1.41	1.35
15	B	1240	CLA	CHC-C1C	2.62	1.41	1.35
15	A	1127	CLA	CHC-C1C	2.62	1.41	1.35
15	A	1132	CLA	CHC-C1C	2.62	1.41	1.35
15	A	1105	CLA	CHC-C1C	2.61	1.41	1.35
15	B	1236	CLA	C3B-C2B	-2.61	1.36	1.40
15	A	1112	CLA	C1B-NB	2.61	1.37	1.35
15	3	611	CLA	CHC-C1C	2.61	1.41	1.35
15	B	1215	CLA	CHC-C1C	2.61	1.41	1.35
15	3	601	CLA	C1B-NB	2.61	1.37	1.35
15	3	610	CLA	CHC-C1C	2.61	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1235	CLA	C1B-NB	2.60	1.37	1.35
15	B	1230	CLA	C1B-NB	2.60	1.37	1.35
15	3	601	CLA	C3B-C2B	-2.59	1.36	1.40
15	A	1129	CLA	CHC-C1C	2.59	1.41	1.35
15	F	1302	CLA	C3B-C2B	-2.59	1.36	1.40
15	B	1202	CLA	CHC-C1C	2.59	1.41	1.35
15	A	1123	CLA	C3B-C2B	-2.59	1.36	1.40
15	A	1112	CLA	CHC-C1C	2.59	1.41	1.35
15	4	607	CLA	C1C-C2C	2.59	1.49	1.44
15	A	1115	CLA	C1B-NB	2.59	1.37	1.35
15	4	603	CLA	C1B-NB	2.59	1.37	1.35
15	A	1138	CLA	C3B-C2B	-2.59	1.36	1.40
15	B	1210	CLA	MG-NC	2.59	2.12	2.06
15	2	603	CLA	C3B-C2B	-2.59	1.36	1.40
15	A	1131	CLA	CHC-C1C	2.58	1.41	1.35
15	A	1136	CLA	CHC-C1C	2.58	1.41	1.35
15	B	1222	CLA	CHC-C1C	2.58	1.41	1.35
15	B	1235	CLA	C1C-NC	-2.58	1.34	1.37
15	3	610	CLA	C1B-NB	2.58	1.37	1.35
15	2	601	CLA	MG-NC	2.58	2.12	2.06
15	B	1227	CLA	CHC-C1C	2.57	1.41	1.35
15	A	1139	CLA	C3B-C2B	-2.57	1.36	1.40
15	2	602	CLA	C1B-NB	2.57	1.37	1.35
15	A	1132	CLA	C1B-NB	2.57	1.37	1.35
15	A	1013	CLA	CHC-C1C	2.57	1.41	1.35
15	2	612	CLA	C1B-NB	2.57	1.37	1.35
15	B	1213	CLA	CHC-C1C	2.57	1.41	1.35
15	A	1102	CLA	CHC-C1C	2.57	1.41	1.35
15	B	1219	CLA	C1B-NB	2.57	1.37	1.35
15	B	1215	CLA	C3B-C2B	-2.57	1.36	1.40
15	1	605	CLA	CHC-C1C	2.57	1.41	1.35
15	1	605	CLA	MG-NC	2.56	2.12	2.06
24	A	1011	CL0	C1C-NC	-2.56	1.34	1.37
15	A	1122	CLA	C3B-C2B	-2.56	1.36	1.40
15	B	1216	CLA	MG-NC	2.56	2.12	2.06
15	2	612	CLA	C3B-C2B	-2.56	1.36	1.40
15	B	1216	CLA	CHC-C1C	2.56	1.41	1.35
15	A	1114	CLA	CHC-C1C	2.56	1.41	1.35
15	4	604	CLA	C1C-C2C	2.56	1.49	1.44
15	1	615	CLA	CHC-C1C	2.56	1.41	1.35
15	4	612	CLA	C1B-NB	2.55	1.37	1.35
15	2	612	CLA	CHC-C1C	2.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1236	CLA	C1C-NC	-2.55	1.34	1.37
15	A	1119	CLA	C3B-C2B	-2.55	1.36	1.40
15	B	1224	CLA	C3B-C2B	-2.55	1.36	1.40
15	2	603	CLA	CHC-C1C	2.54	1.41	1.35
21	2	811	DGD	CAA-C9A	-2.54	1.33	1.51
15	3	610	CLA	C3B-C2B	-2.54	1.36	1.40
15	4	608	CLA	CHC-C1C	2.54	1.41	1.35
15	B	1236	CLA	CHC-C1C	2.54	1.41	1.35
15	4	602	CLA	MG-NC	2.54	2.12	2.06
21	4	811	DGD	O5D-C1E	2.54	1.44	1.40
15	2	615	CLA	C1B-NB	2.53	1.37	1.35
15	1	608	CLA	C1B-NB	2.53	1.37	1.35
15	A	1107	CLA	CHC-C1C	2.53	1.41	1.35
15	4	606	CLA	CHC-C1C	2.53	1.41	1.35
15	B	1219	CLA	C1C-C2C	2.53	1.49	1.44
15	B	1211	CLA	CHC-C1C	2.52	1.41	1.35
15	B	1219	CLA	MG-NC	2.52	2.12	2.06
15	A	1130	CLA	C3B-C2B	-2.52	1.36	1.40
15	4	604	CLA	C1C-NC	-2.52	1.34	1.37
15	A	1123	CLA	C1C-C2C	2.52	1.49	1.44
15	B	1221	CLA	CHC-C1C	2.51	1.41	1.35
15	4	606	CLA	C1B-NB	2.51	1.37	1.35
15	A	1113	CLA	C3B-C2B	-2.51	1.36	1.40
15	3	601	CLA	C1C-C2C	2.51	1.49	1.44
15	J	1302	CLA	CHC-C1C	2.51	1.41	1.35
15	4	615	CLA	CHC-C1C	2.51	1.41	1.35
16	2	610	CHL	C4B-NB	2.51	1.37	1.35
15	A	1137	CLA	C1B-NB	2.51	1.37	1.35
15	1	615	CLA	C3B-C2B	-2.51	1.36	1.40
15	B	1202	CLA	C1B-NB	2.51	1.37	1.35
15	B	1204	CLA	C3B-C2B	-2.51	1.36	1.40
15	B	1223	CLA	C1C-C2C	2.50	1.49	1.44
15	1	611	CLA	CHC-C1C	2.50	1.41	1.35
15	2	604	CLA	CHC-C1C	2.50	1.41	1.35
15	A	1103	CLA	CHC-C1C	2.50	1.41	1.35
15	B	1202	CLA	C1C-C2C	2.49	1.49	1.44
15	A	1140	CLA	C3B-C2B	-2.49	1.36	1.40
15	A	1137	CLA	C3B-C2B	-2.49	1.36	1.40
15	4	603	CLA	MG-NC	2.49	2.12	2.06
15	A	1106	CLA	C1B-NB	2.48	1.37	1.35
15	A	1115	CLA	C1C-C2C	2.48	1.49	1.44
15	A	1120	CLA	C3B-C2B	-2.48	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	606	CLA	MG-NC	2.48	2.12	2.06
15	2	602	CLA	C3B-C2B	-2.48	1.36	1.40
15	4	601	CLA	MG-NC	2.48	2.12	2.06
15	B	1228	CLA	C1C-NC	-2.47	1.34	1.37
15	3	603	CLA	CHC-C1C	2.47	1.41	1.35
15	4	615	CLA	C1B-NB	2.47	1.37	1.35
15	B	1236	CLA	MG-NC	2.47	2.12	2.06
15	B	1215	CLA	C1C-C2C	2.46	1.49	1.44
15	B	1023	CLA	C1C-C2C	2.46	1.49	1.44
15	A	1118	CLA	C1B-NB	2.46	1.37	1.35
15	2	606	CLA	C1B-NB	2.46	1.37	1.35
15	B	1240	CLA	C3B-C2B	-2.46	1.37	1.40
15	A	1107	CLA	C3B-C2B	-2.46	1.37	1.40
15	B	1225	CLA	C3B-C2B	-2.46	1.37	1.40
13	2	502	XAT	O24-C25	-2.46	1.42	1.46
16	4	613	CHL	C3B-C2B	-2.46	1.37	1.40
15	B	1208	CLA	CHC-C1C	2.46	1.41	1.35
15	4	602	CLA	C3B-C2B	-2.45	1.37	1.40
15	3	611	CLA	C3B-C2B	-2.45	1.37	1.40
15	A	1106	CLA	CHC-C1C	2.45	1.41	1.35
15	A	1116	CLA	C1B-NB	2.45	1.37	1.35
15	B	1238	CLA	C3B-C2B	-2.45	1.37	1.40
15	B	1221	CLA	C3B-C2B	-2.45	1.37	1.40
15	A	1113	CLA	C1B-NB	2.45	1.37	1.35
15	3	615	CLA	CHC-C1C	2.45	1.41	1.35
15	B	1239	CLA	C3B-C2B	-2.45	1.37	1.40
15	A	1141	CLA	C3B-C2B	-2.45	1.37	1.40
15	A	1128	CLA	MG-NC	2.45	2.12	2.06
13	1	502	XAT	O24-C25	-2.45	1.42	1.46
15	A	1126	CLA	C1B-NB	2.44	1.37	1.35
15	3	615	CLA	C3B-C2B	-2.44	1.37	1.40
15	4	603	CLA	CHC-C1C	2.44	1.41	1.35
15	B	1213	CLA	MG-NC	2.44	2.12	2.06
24	A	1011	CL0	C1B-CHB	2.44	1.47	1.41
15	2	607	CLA	C3B-C2B	-2.44	1.37	1.40
15	B	1022	CLA	MG-NC	2.44	2.12	2.06
15	A	1131	CLA	C3B-C2B	-2.43	1.37	1.40
15	1	601	CLA	MG-NC	2.43	2.12	2.06
15	2	605	CLA	C3B-C2B	-2.43	1.37	1.40
15	B	1236	CLA	C1B-NB	2.43	1.37	1.35
15	A	1128	CLA	C3B-C2B	-2.43	1.37	1.40
15	B	1209	CLA	C3B-C2B	-2.43	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1108	CLA	C1C-C2C	2.42	1.49	1.44
15	B	1214	CLA	C3B-C2B	-2.42	1.37	1.40
15	B	1226	CLA	MG-NC	2.42	2.12	2.06
15	4	612	CLA	MG-NC	2.42	2.12	2.06
15	2	603	CLA	C1B-NB	2.42	1.37	1.35
15	A	1130	CLA	C1B-NB	2.41	1.37	1.35
15	1	601	CLA	C1B-NB	2.41	1.37	1.35
15	B	1223	CLA	C4B-NB	-2.41	1.33	1.35
15	3	608	CLA	C3B-C2B	-2.41	1.37	1.40
15	A	1106	CLA	C3B-C2B	-2.41	1.37	1.40
15	B	1208	CLA	C3B-C2B	-2.41	1.37	1.40
15	F	1302	CLA	MG-NC	2.41	2.12	2.06
15	B	1230	CLA	CHC-C1C	2.41	1.41	1.35
15	B	1228	CLA	C3B-C2B	-2.41	1.37	1.40
15	A	1108	CLA	C1B-NB	2.41	1.37	1.35
15	3	607	CLA	C1B-NB	2.40	1.37	1.35
15	A	1135	CLA	C3B-C2B	-2.40	1.37	1.40
15	3	615	CLA	C1B-NB	2.40	1.37	1.35
15	B	1217	CLA	C3B-C2B	-2.40	1.37	1.40
15	2	603	CLA	MG-NC	2.39	2.12	2.06
15	A	1125	CLA	C1B-NB	2.39	1.37	1.35
15	2	605	CLA	C1C-C2C	2.39	1.49	1.44
15	B	1237	CLA	C1B-NB	2.39	1.37	1.35
15	A	1136	CLA	C1B-NB	2.39	1.37	1.35
15	A	1133	CLA	C3B-C2B	-2.39	1.37	1.40
15	A	1127	CLA	C3B-C2B	-2.39	1.37	1.40
15	A	1119	CLA	C1B-NB	2.38	1.37	1.35
15	2	604	CLA	MG-NC	2.38	2.11	2.06
15	B	1238	CLA	C1B-NB	2.38	1.37	1.35
15	3	607	CLA	C3B-C2B	-2.38	1.37	1.40
15	4	603	CLA	C3B-C2B	-2.38	1.37	1.40
15	4	604	CLA	C3B-C2B	-2.38	1.37	1.40
15	A	1134	CLA	C1B-NB	2.38	1.37	1.35
15	A	1118	CLA	C3B-C2B	-2.38	1.37	1.40
15	B	1209	CLA	C1B-NB	2.37	1.37	1.35
15	B	1021	CLA	C1B-NB	2.37	1.37	1.35
15	1	613	CLA	C3B-C2B	-2.37	1.37	1.40
15	A	1121	CLA	C3B-C2B	-2.37	1.37	1.40
15	B	1222	CLA	C3B-C2B	-2.37	1.37	1.40
15	A	1110	CLA	C1C-C2C	2.37	1.49	1.44
22	2	821	LMT	O3'-C3'	-2.37	1.37	1.43
15	A	1103	CLA	C3B-C2B	-2.36	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1101	CLA	C1B-NB	2.36	1.37	1.35
21	2	811	DGD	O3G-C1D	2.36	1.44	1.40
15	3	603	CLA	MG-NC	2.36	2.11	2.06
15	A	1119	CLA	C1C-C2C	2.36	1.49	1.44
15	3	613	CLA	C1C-C2C	2.36	1.49	1.44
15	B	1216	CLA	C3B-C2B	-2.36	1.37	1.40
15	4	615	CLA	C3B-C2B	-2.36	1.37	1.40
15	4	605	CLA	C1B-NB	2.36	1.37	1.35
15	A	1102	CLA	C1B-NB	2.35	1.37	1.35
15	3	612	CLA	C3B-C2B	-2.35	1.37	1.40
15	A	1012	CLA	C1C-C2C	2.35	1.49	1.44
15	2	607	CLA	C1B-NB	2.35	1.37	1.35
15	1	612	CLA	C1B-NB	2.35	1.37	1.35
15	B	1218	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1215	CLA	C1B-NB	2.35	1.37	1.35
15	2	608	CLA	C3B-C2B	-2.35	1.37	1.40
15	A	1120	CLA	C1C-C2C	2.35	1.49	1.44
15	B	1234	CLA	C3B-C2B	-2.35	1.37	1.40
15	A	1101	CLA	C3B-C2B	-2.35	1.37	1.40
15	B	1201	CLA	C3B-C2B	-2.34	1.37	1.40
15	B	1221	CLA	C1C-C2C	2.34	1.49	1.44
15	A	1013	CLA	MG-NC	2.34	2.11	2.06
15	2	604	CLA	C3B-C2B	-2.34	1.37	1.40
15	B	1210	CLA	C3B-C2B	-2.34	1.37	1.40
15	2	606	CLA	C1C-C2C	2.34	1.49	1.44
15	J	1302	CLA	C1B-NB	2.33	1.37	1.35
15	B	1023	CLA	C1C-NC	-2.33	1.34	1.37
22	2	821	LMT	O2B-C2B	-2.33	1.37	1.43
15	3	605	CLA	C3B-C2B	-2.33	1.37	1.40
15	A	1121	CLA	C1C-C2C	2.33	1.49	1.44
15	2	612	CLA	C1C-C2C	2.33	1.49	1.44
15	4	607	CLA	MG-NC	2.32	2.11	2.06
15	A	1114	CLA	C3B-C2B	-2.32	1.37	1.40
15	1	615	CLA	C1C-C2C	2.32	1.49	1.44
15	A	1114	CLA	C1B-NB	2.32	1.37	1.35
15	B	1240	CLA	C1B-NB	2.32	1.37	1.35
15	B	1239	CLA	C1C-C2C	2.32	1.49	1.44
15	B	1235	CLA	C3B-C2B	-2.31	1.37	1.40
15	3	605	CLA	MG-NC	2.31	2.11	2.06
15	2	607	CLA	C1C-C2C	2.31	1.49	1.44
15	A	1109	CLA	C3B-C2B	-2.31	1.37	1.40
15	B	1214	CLA	C1A-CHA	2.31	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1206	CLA	C1C-C2C	2.31	1.49	1.44
15	2	602	CLA	C1C-C2C	2.31	1.49	1.44
15	A	1012	CLA	C1B-NB	2.31	1.37	1.35
15	4	609	CLA	C3B-C2B	-2.31	1.37	1.40
15	3	603	CLA	C3B-C2B	-2.30	1.37	1.40
15	A	1124	CLA	C1B-NB	2.30	1.37	1.35
15	B	1219	CLA	C3B-C2B	-2.30	1.37	1.40
15	B	1240	CLA	C1C-C2C	2.30	1.49	1.44
15	3	612	CLA	MG-NC	2.30	2.11	2.06
15	3	603	CLA	C1A-CHA	2.30	1.52	1.43
15	2	615	CLA	C1C-C2C	2.29	1.49	1.44
15	B	1023	CLA	C3B-C2B	-2.29	1.37	1.40
15	B	1217	CLA	MG-NC	2.29	2.11	2.06
22	2	821	LMT	O3B-C3B	-2.29	1.37	1.43
15	B	1206	CLA	C3B-C2B	-2.29	1.37	1.40
15	1	606	CLA	C1B-NB	2.29	1.37	1.35
15	A	1105	CLA	C1C-C2C	2.29	1.49	1.44
15	A	1117	CLA	MG-NC	2.28	2.11	2.06
15	B	1201	CLA	C1B-NB	2.28	1.37	1.35
22	2	821	LMT	O2'-C2'	-2.28	1.37	1.43
15	B	1205	CLA	C1B-NB	2.28	1.37	1.35
15	3	608	CLA	C1B-NB	2.28	1.37	1.35
15	A	1120	CLA	C1B-NB	2.28	1.37	1.35
15	B	1232	CLA	C3B-C2B	-2.28	1.37	1.40
15	1	607	CLA	C3B-C2B	-2.28	1.37	1.40
15	A	1123	CLA	C1B-NB	2.28	1.37	1.35
15	A	1109	CLA	C1C-C2C	2.28	1.49	1.44
15	B	1207	CLA	C4B-NB	-2.28	1.33	1.35
15	B	1224	CLA	C1C-C2C	2.27	1.49	1.44
15	3	607	CLA	C1C-C2C	2.27	1.49	1.44
15	B	1227	CLA	C1B-NB	2.27	1.37	1.35
15	4	612	CLA	C3B-C2B	-2.27	1.37	1.40
15	1	612	CLA	C3B-C2B	-2.27	1.37	1.40
15	B	1220	CLA	C1B-NB	2.27	1.37	1.35
15	A	1102	CLA	MG-NC	2.27	2.11	2.06
15	A	1104	CLA	C3B-C2B	-2.27	1.37	1.40
15	B	1225	CLA	MG-NC	2.26	2.11	2.06
15	1	605	CLA	C3B-C2B	-2.26	1.37	1.40
15	B	1229	CLA	C4B-NB	-2.26	1.33	1.35
23	B	5031	GSH	O2-C2	-2.26	1.18	1.23
15	A	1114	CLA	C1C-C2C	2.26	1.48	1.44
15	A	1134	CLA	C1C-C2C	2.26	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	610	CLA	C1C-C2C	2.26	1.48	1.44
15	A	1140	CLA	CHC-C1C	2.25	1.40	1.35
15	A	1125	CLA	C3B-C2B	-2.25	1.37	1.40
15	B	1205	CLA	C3B-C2B	-2.25	1.37	1.40
15	B	1234	CLA	C1A-CHA	2.25	1.52	1.43
15	A	1129	CLA	C3B-C2B	-2.25	1.37	1.40
15	1	607	CLA	MG-NC	2.25	2.11	2.06
15	A	1130	CLA	C1C-C2C	2.25	1.48	1.44
15	A	1112	CLA	C3B-C2B	-2.25	1.37	1.40
15	B	1021	CLA	C3B-C2B	-2.25	1.37	1.40
15	B	1222	CLA	C1B-NB	2.24	1.37	1.35
15	A	1140	CLA	C1C-C2C	2.24	1.48	1.44
15	A	1124	CLA	C3B-C2B	-2.24	1.37	1.40
23	4	831	GSH	O2-C2	-2.24	1.18	1.23
15	A	1134	CLA	C3B-C2B	-2.24	1.37	1.40
15	A	1012	CLA	MG-NC	2.24	2.11	2.06
15	2	608	CLA	C1C-C2C	2.24	1.48	1.44
15	A	1124	CLA	C1C-C2C	2.24	1.48	1.44
15	3	605	CLA	C1B-NB	2.23	1.37	1.35
15	B	1217	CLA	C1B-NB	2.23	1.37	1.35
15	A	1133	CLA	C1C-C2C	2.23	1.48	1.44
15	B	1212	CLA	C3B-C2B	-2.23	1.37	1.40
15	B	1238	CLA	C1C-C2C	2.23	1.48	1.44
15	J	1302	CLA	MG-NC	2.23	2.11	2.06
15	1	604	CLA	C1B-NB	2.23	1.37	1.35
15	1	613	CLA	C1C-C2C	2.22	1.48	1.44
15	B	1237	CLA	C3B-C2B	-2.22	1.37	1.40
15	A	1103	CLA	C1B-NB	2.22	1.37	1.35
15	A	1108	CLA	C3B-C2B	-2.22	1.37	1.40
15	1	603	CLA	C1A-CHA	2.21	1.52	1.43
14	J	4002	BCR	C1-C6	-2.21	1.50	1.53
15	B	1021	CLA	C1C-C2C	2.21	1.48	1.44
15	B	1235	CLA	CHC-C1C	2.21	1.40	1.35
15	A	1110	CLA	C3B-C2B	-2.21	1.37	1.40
15	1	612	CLA	MG-NC	2.21	2.11	2.06
15	3	605	CLA	C1C-C2C	2.21	1.48	1.44
15	4	608	CLA	C3B-C2B	-2.21	1.37	1.40
15	4	603	CLA	C1C-C2C	2.20	1.48	1.44
15	B	1232	CLA	C1C-C2C	2.20	1.48	1.44
15	A	1131	CLA	C1B-NB	2.20	1.37	1.35
15	1	604	CLA	C3B-C2B	-2.20	1.37	1.40
15	A	1127	CLA	C1B-NB	2.20	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1203	CLA	C1B-NB	2.20	1.37	1.35
15	4	606	CLA	C3B-C2B	-2.20	1.37	1.40
15	A	1127	CLA	C1C-C2C	2.20	1.48	1.44
15	1	603	CLA	C3B-C2B	-2.20	1.37	1.40
15	A	1103	CLA	C1C-C2C	2.20	1.48	1.44
15	B	1227	CLA	MG-NC	2.20	2.11	2.06
15	B	1205	CLA	MG-NC	2.20	2.11	2.06
15	4	604	CLA	C1B-NB	2.19	1.37	1.35
15	J	1302	CLA	C3B-C2B	-2.19	1.37	1.40
15	A	1122	CLA	C1C-C2C	2.19	1.48	1.44
15	A	1138	CLA	C1B-NB	2.19	1.37	1.35
15	A	1116	CLA	C3B-C2B	-2.19	1.37	1.40
15	A	1106	CLA	C1C-C2C	2.18	1.48	1.44
15	3	608	CLA	C1C-C2C	2.18	1.48	1.44
17	A	5001	LHG	O7-C7	-2.18	1.34	1.42
15	B	1204	CLA	C1C-C2C	2.18	1.48	1.44
15	A	1132	CLA	C1C-C2C	2.18	1.48	1.44
15	A	1129	CLA	C1B-NB	2.18	1.37	1.35
15	B	1222	CLA	C1C-C2C	2.18	1.48	1.44
15	A	1141	CLA	C1B-NB	2.18	1.37	1.35
15	1	602	CLA	C3B-C2B	-2.18	1.37	1.40
15	4	608	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1211	CLA	C1C-C2C	2.18	1.48	1.44
15	B	1212	CLA	C1B-NB	2.17	1.37	1.35
15	B	1205	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1116	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1121	CLA	C1B-NB	2.17	1.37	1.35
15	A	1115	CLA	C3B-C2B	-2.17	1.37	1.40
15	A	1104	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1141	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1013	CLA	C1A-CHA	2.17	1.52	1.43
15	A	1136	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1131	CLA	MG-NC	2.17	2.11	2.06
15	A	1105	CLA	MG-NC	2.17	2.11	2.06
15	B	1201	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1209	CLA	C1C-C2C	2.16	1.48	1.44
15	4	602	CLA	C1B-NB	2.16	1.37	1.35
15	3	603	CLA	C1B-NB	2.16	1.37	1.35
15	B	1235	CLA	MG-NC	2.16	2.11	2.06
15	A	1104	CLA	MG-NC	2.16	2.11	2.06
15	A	1113	CLA	C1C-C2C	2.16	1.48	1.44
15	A	1104	CLA	C1B-NB	2.16	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1138	CLA	C1C-C2C	2.16	1.48	1.44
15	F	1301	CLA	C1D-C2D	2.16	1.47	1.42
15	1	602	CLA	C1C-C2C	2.16	1.48	1.44
15	4	601	CLA	C1A-CHA	2.16	1.52	1.43
15	1	604	CLA	C1C-C2C	2.16	1.48	1.44
15	1	611	CLA	C1C-C2C	2.16	1.48	1.44
15	B	1221	CLA	C1A-CHA	2.16	1.52	1.43
15	A	1137	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1204	CLA	C1B-NB	2.15	1.37	1.35
15	A	1139	CLA	C1C-C2C	2.15	1.48	1.44
15	A	1118	CLA	C1C-C2C	2.15	1.48	1.44
15	B	1234	CLA	MG-NC	2.15	2.11	2.06
15	B	1226	CLA	C3B-C2B	-2.15	1.37	1.40
15	A	1127	CLA	MG-NC	2.15	2.11	2.06
15	B	1023	CLA	MG-NC	2.15	2.11	2.06
15	A	1136	CLA	C3B-C2B	-2.15	1.37	1.40
15	1	602	CLA	MG-NC	2.15	2.11	2.06
15	4	605	CLA	C1C-C2C	2.15	1.48	1.44
16	4	610	CHL	C4B-NB	2.15	1.37	1.35
15	3	610	CLA	MG-NC	2.15	2.11	2.06
15	4	607	CLA	C3B-C2B	-2.15	1.37	1.40
15	A	1122	CLA	C1B-NB	2.15	1.37	1.35
15	B	1223	CLA	C1B-NB	2.15	1.37	1.35
16	4	610	CHL	C3B-C2B	-2.14	1.37	1.40
15	4	604	CLA	C1D-C2D	2.14	1.47	1.42
15	2	606	CLA	C1A-CHA	2.14	1.52	1.43
15	3	615	CLA	C1A-CHA	2.14	1.52	1.43
15	2	615	CLA	MG-NC	2.14	2.11	2.06
15	B	1208	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1213	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1131	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1140	CLA	C1A-CHA	2.13	1.52	1.43
15	A	1129	CLA	C1C-C2C	2.13	1.48	1.44
15	3	606	CLA	C1C-C2C	2.13	1.48	1.44
15	A	1125	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1226	CLA	C1C-C2C	2.13	1.48	1.44
15	4	612	CLA	C1A-CHA	2.13	1.51	1.43
15	B	1230	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1228	CLA	MG-NC	2.13	2.11	2.06
15	A	1112	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1206	CLA	MG-NC	2.12	2.11	2.06
15	A	1132	CLA	MG-NC	2.12	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1224	CLA	MG-NC	2.12	2.11	2.06
15	A	1135	CLA	MG-NC	2.12	2.11	2.06
15	B	1237	CLA	C1C-C2C	2.12	1.48	1.44
15	F	1302	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1212	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1204	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1235	CLA	C1A-CHA	2.12	1.51	1.43
15	A	1107	CLA	C1C-C2C	2.12	1.48	1.44
15	B	1217	CLA	C1C-C2C	2.12	1.48	1.44
15	1	613	CLA	MG-NC	2.11	2.11	2.06
15	A	1101	CLA	C1C-C2C	2.11	1.48	1.44
15	A	1114	CLA	C1A-CHA	2.11	1.51	1.43
15	3	606	CLA	C3B-C2B	-2.11	1.37	1.40
12	4	501	LUT	C1-C6	-2.11	1.50	1.53
15	3	612	CLA	C1B-NB	2.11	1.37	1.35
15	A	1132	CLA	C3B-C2B	-2.11	1.37	1.40
15	2	605	CLA	C1B-NB	2.11	1.37	1.35
15	4	608	CLA	MG-NC	2.11	2.11	2.06
15	A	1111	CLA	C1B-NB	2.11	1.37	1.35
15	1	603	CLA	C1B-NB	2.11	1.37	1.35
15	1	613	CLA	C1A-CHA	2.10	1.51	1.43
15	B	1239	CLA	C1A-CHA	2.10	1.51	1.43
15	1	601	CLA	C1C-C2C	2.10	1.48	1.44
15	B	1203	CLA	C3B-C2B	-2.10	1.37	1.40
15	1	602	CLA	C1B-NB	2.10	1.37	1.35
15	1	615	CLA	C1B-NB	2.10	1.37	1.35
15	4	609	CLA	C1A-CHA	2.10	1.51	1.43
15	A	1122	CLA	MG-NC	2.10	2.11	2.06
15	A	1140	CLA	MG-NC	2.10	2.11	2.06
15	B	1235	CLA	C1C-C2C	2.10	1.48	1.44
15	A	1112	CLA	MG-NC	2.10	2.11	2.06
15	B	1218	CLA	C1A-CHA	2.10	1.51	1.43
15	B	1203	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1218	CLA	C3B-C2B	-2.09	1.37	1.40
15	B	1231	CLA	C3B-C2B	-2.09	1.37	1.40
15	3	606	CLA	C1B-NB	2.09	1.37	1.35
15	B	1218	CLA	MG-NC	2.09	2.11	2.06
15	A	1110	CLA	C1B-NB	2.09	1.37	1.35
15	1	603	CLA	C4B-NB	-2.09	1.33	1.35
16	2	609	CHL	C3B-C2B	-2.09	1.37	1.40
15	A	1108	CLA	C1A-CHA	2.09	1.51	1.43
15	B	1236	CLA	C1A-CHA	2.09	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	607	CLA	C1A-CHA	2.08	1.51	1.43
15	4	612	CLA	C1C-C2C	2.08	1.48	1.44
15	B	1230	CLA	C3B-C2B	-2.08	1.37	1.40
15	A	1113	CLA	MG-NC	2.08	2.11	2.06
15	A	1111	CLA	C3B-C2B	-2.08	1.37	1.40
15	B	1211	CLA	C1A-CHA	2.08	1.51	1.43
15	B	1214	CLA	C1C-C2C	2.08	1.48	1.44
15	F	1302	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1103	CLA	C1A-CHA	2.07	1.51	1.43
15	B	1213	CLA	C3B-C2B	-2.07	1.37	1.40
15	2	608	CLA	C1B-NB	2.07	1.37	1.35
15	A	1128	CLA	C1B-NB	2.07	1.37	1.35
15	2	612	CLA	MG-NC	2.07	2.11	2.06
15	A	1102	CLA	C1A-CHA	2.07	1.51	1.43
13	3	502	XAT	O24-C25	-2.07	1.43	1.46
15	A	1128	CLA	C1A-CHA	2.07	1.51	1.43
15	2	604	CLA	C1A-CHA	2.06	1.51	1.43
15	B	1222	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1116	CLA	MG-NC	2.06	2.11	2.06
15	B	1214	CLA	C1B-NB	2.06	1.37	1.35
15	B	1227	CLA	C1A-CHA	2.06	1.51	1.43
15	2	601	CLA	C1B-NB	2.06	1.37	1.35
24	A	1011	CL0	C1B-NB	-2.06	1.33	1.35
15	B	1220	CLA	MG-NC	2.06	2.11	2.06
15	B	1219	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1134	CLA	C1A-CHA	2.06	1.51	1.43
15	A	1135	CLA	C1C-C2C	2.06	1.48	1.44
15	1	604	CLA	MG-NC	2.06	2.11	2.06
15	A	1118	CLA	MG-NC	2.05	2.11	2.06
15	A	1132	CLA	C1A-CHA	2.05	1.51	1.43
15	A	1117	CLA	C1A-CHA	2.05	1.51	1.43
15	A	1117	CLA	C1B-NB	2.05	1.37	1.35
15	B	1201	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1232	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1023	CLA	C1D-C2D	2.05	1.47	1.42
15	2	605	CLA	C1A-CHA	2.05	1.51	1.43
15	A	1106	CLA	C1A-CHA	2.05	1.51	1.43
15	1	606	CLA	C1C-C2C	2.05	1.48	1.44
15	A	1102	CLA	C3B-C2B	-2.05	1.37	1.40
15	A	1126	CLA	C3B-C2B	-2.04	1.37	1.40
15	B	1229	CLA	C1C-C2C	2.04	1.48	1.44
16	4	611	CHL	CHC-C1C	2.04	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	606	CLA	C1A-CHA	2.04	1.51	1.43
15	2	608	CLA	MG-NC	2.04	2.11	2.06
15	A	1115	CLA	C1A-CHA	2.04	1.51	1.43
15	1	615	CLA	C1A-CHA	2.04	1.51	1.43
23	4	831	GSH	OE1-CD1	-2.03	1.19	1.23
15	B	1216	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1209	CLA	MG-NC	2.03	2.11	2.06
15	A	1113	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1021	CLA	C1A-CHA	2.03	1.51	1.43
15	A	1120	CLA	C1A-CHA	2.03	1.51	1.43
15	2	615	CLA	C3B-C2B	-2.03	1.37	1.40
15	A	1105	CLA	C1A-CHA	2.03	1.51	1.43
15	A	1109	CLA	C1B-NB	2.03	1.37	1.35
15	A	1109	CLA	C1A-CHA	2.03	1.51	1.43
15	1	603	CLA	MG-NC	2.03	2.11	2.06
15	A	1135	CLA	C1A-CHA	2.03	1.51	1.43
15	3	603	CLA	C1C-C2C	2.02	1.48	1.44
15	4	608	CLA	C1B-NB	2.02	1.37	1.35
15	3	608	CLA	C1A-CHA	2.02	1.51	1.43
15	1	601	CLA	C1A-CHA	2.02	1.51	1.43
15	3	611	CLA	C1C-C2C	2.02	1.48	1.44
15	B	1213	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1118	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1121	CLA	C1A-CHA	2.02	1.51	1.43
15	B	1225	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1133	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1110	CLA	MG-NC	2.02	2.11	2.06
15	3	612	CLA	C1A-CHA	2.02	1.51	1.43
15	B	1214	CLA	MG-NC	2.02	2.11	2.06
15	B	1237	CLA	C1A-CHA	2.02	1.51	1.43
15	A	1123	CLA	C1A-CHA	2.02	1.51	1.43
15	3	607	CLA	C1A-CHA	2.01	1.51	1.43
15	A	1114	CLA	MG-NC	2.01	2.11	2.06
15	B	1218	CLA	C1B-NB	2.01	1.37	1.35
15	B	1211	CLA	MG-NC	2.01	2.11	2.06
15	2	615	CLA	C1A-CHA	2.01	1.51	1.43
15	B	1206	CLA	C1A-CHA	2.01	1.51	1.43
15	B	1205	CLA	C1A-CHA	2.01	1.51	1.43
22	2	821	LMT	O4'-C4B	-2.01	1.38	1.43
15	1	611	CLA	C1A-CHA	2.01	1.51	1.43
15	1	602	CLA	C1A-CHA	2.01	1.51	1.43
15	A	1107	CLA	C1B-NB	2.01	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1228	CLA	C1A-CHA	2.01	1.51	1.43
21	B	5002	DGD	O5D-C1E	2.01	1.43	1.40
15	1	608	CLA	C1C-C2C	2.01	1.48	1.44
15	1	612	CLA	C1C-C2C	2.01	1.48	1.44
15	B	1201	CLA	MG-NC	2.01	2.11	2.06
15	B	1211	CLA	C3B-C2B	-2.00	1.37	1.40
15	B	1230	CLA	MG-NC	2.00	2.11	2.06
15	A	1137	CLA	MG-NC	2.00	2.11	2.06
15	2	606	CLA	C3B-C2B	-2.00	1.37	1.40
15	2	601	CLA	C1A-CHA	2.00	1.51	1.43
15	4	604	CLA	C1A-CHA	2.00	1.51	1.43
15	3	608	CLA	MG-NC	2.00	2.11	2.06
15	B	1207	CLA	C2A-C1A	-2.00	1.40	1.52
15	B	1022	CLA	C1C-C2C	2.00	1.48	1.44
15	A	1124	CLA	C1A-CHA	2.00	1.51	1.43

All (1854) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4001	BCR	C10-C11-C12	17.73	178.54	123.22
14	2	503	BCR	C10-C11-C12	17.71	178.50	123.22
14	3	504	BCR	C10-C11-C12	17.63	178.23	123.22
14	4	503	BCR	C10-C11-C12	17.61	178.18	123.22
14	A	4004	BCR	C10-C11-C12	17.60	178.13	123.22
14	F	4002	BCR	C10-C11-C12	17.57	178.04	123.22
14	A	4007	BCR	C10-C11-C12	17.54	177.94	123.22
14	B	4006	BCR	C10-C11-C12	17.46	177.72	123.22
14	4	505	BCR	C10-C11-C12	17.46	177.70	123.22
14	A	4002	BCR	C10-C11-C12	17.40	177.53	123.22
14	B	4005	BCR	C10-C11-C12	17.39	177.50	123.22
14	3	503	BCR	C10-C11-C12	17.24	177.01	123.22
14	B	4004	BCR	C10-C11-C12	17.23	176.99	123.22
14	1	505	BCR	C10-C11-C12	17.11	176.63	123.22
14	B	4002	BCR	C10-C11-C12	16.84	175.77	123.22
14	B	4003	BCR	C10-C11-C12	16.71	175.38	123.22
14	J	4003	BCR	C10-C11-C12	16.69	175.32	123.22
14	J	4001	BCR	C10-C11-C12	16.64	175.13	123.22
14	A	4006	BCR	C10-C11-C12	16.56	174.90	123.22
14	1	505	BCR	C16-C15-C14	16.50	157.27	123.47
14	1	503	BCR	C10-C11-C12	16.45	174.55	123.22
14	A	4003	BCR	C10-C11-C12	16.44	174.54	123.22
12	1	501	LUT	C36-C21-C26	-16.44	84.64	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	4002	BCR	C10-C11-C12	16.43	174.48	123.22
14	A	4007	BCR	C16-C15-C14	16.10	156.46	123.47
14	3	504	BCR	C16-C15-C14	15.85	155.94	123.47
12	1	501	LUT	C37-C21-C36	-15.46	85.11	107.89
14	A	4005	BCR	C16-C15-C14	15.36	154.93	123.47
14	B	4001	BCR	C16-C15-C14	15.33	154.87	123.47
14	F	4002	BCR	C16-C15-C14	14.90	154.00	123.47
14	4	505	BCR	C16-C15-C14	14.75	153.69	123.47
14	2	503	BCR	C16-C15-C14	14.69	153.56	123.47
14	J	4002	BCR	C16-C15-C14	14.68	153.55	123.47
14	B	4003	BCR	C11-C10-C9	14.48	147.97	127.31
14	1	503	BCR	C16-C15-C14	14.46	153.09	123.47
14	B	4002	BCR	C16-C15-C14	14.33	152.84	123.47
14	B	4005	BCR	C16-C15-C14	14.33	152.82	123.47
14	A	4003	BCR	C11-C10-C9	14.29	147.70	127.31
14	B	4004	BCR	C11-C10-C9	14.06	147.38	127.31
14	A	4004	BCR	C16-C15-C14	13.94	152.03	123.47
14	A	4007	BCR	C11-C10-C9	13.87	147.11	127.31
14	1	503	BCR	C11-C10-C9	13.80	147.01	127.31
14	3	503	BCR	C11-C10-C9	13.73	146.91	127.31
14	B	4003	BCR	C16-C15-C14	13.65	151.44	123.47
14	4	503	BCR	C16-C15-C14	13.62	151.38	123.47
14	B	4001	BCR	C11-C10-C9	13.62	146.75	127.31
14	B	4006	BCR	C16-C15-C14	13.61	151.36	123.47
14	B	4004	BCR	C16-C15-C14	13.58	151.29	123.47
14	J	4001	BCR	C11-C10-C9	13.48	146.54	127.31
14	A	4006	BCR	C11-C10-C9	13.47	146.54	127.31
14	F	4002	BCR	C11-C10-C9	13.42	146.46	127.31
14	J	4002	BCR	C11-C10-C9	13.40	146.43	127.31
14	4	503	BCR	C11-C10-C9	13.24	146.21	127.31
14	J	4003	BCR	C16-C15-C14	13.23	150.57	123.47
14	B	4005	BCR	C11-C10-C9	13.08	145.97	127.31
14	3	504	BCR	C11-C10-C9	13.01	145.88	127.31
14	2	503	BCR	C11-C10-C9	12.99	145.85	127.31
14	J	4001	BCR	C16-C15-C14	12.95	150.01	123.47
14	A	4002	BCR	C21-C20-C19	12.94	163.61	123.22
14	A	4002	BCR	C16-C15-C14	12.71	149.52	123.47
14	B	4006	BCR	C11-C10-C9	12.67	145.39	127.31
14	4	505	BCR	C21-C20-C19	12.62	162.61	123.22
14	3	503	BCR	C16-C15-C14	12.50	149.07	123.47
14	A	4002	BCR	C11-C10-C9	12.36	144.95	127.31
14	F	4002	BCR	C21-C20-C19	12.29	161.56	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4003	BCR	C21-C20-C19	12.29	161.56	123.22
14	A	4004	BCR	C21-C20-C19	12.27	161.50	123.22
14	A	4004	BCR	C11-C10-C9	12.16	144.67	127.31
14	A	4003	BCR	C16-C15-C14	12.12	148.31	123.47
14	B	4006	BCR	C21-C20-C19	12.08	160.92	123.22
14	B	4002	BCR	C21-C20-C19	12.05	160.81	123.22
14	J	4003	BCR	C11-C12-C13	11.98	160.08	126.42
14	J	4003	BCR	C11-C10-C9	11.93	144.33	127.31
12	1	501	LUT	C36-C21-C22	-11.89	86.92	109.44
14	1	505	BCR	C11-C10-C9	11.85	144.22	127.31
14	1	505	BCR	C21-C20-C19	11.84	160.16	123.22
14	1	503	BCR	C11-C12-C13	11.78	159.51	126.42
14	J	4001	BCR	C11-C12-C13	11.74	159.39	126.42
14	A	4006	BCR	C16-C15-C14	11.72	147.49	123.47
14	J	4003	BCR	C21-C20-C19	11.72	159.79	123.22
14	A	4003	BCR	C11-C12-C13	11.71	159.32	126.42
14	J	4001	BCR	C21-C20-C19	11.70	159.73	123.22
14	4	505	BCR	C11-C10-C9	11.68	143.98	127.31
14	J	4002	BCR	C21-C20-C19	11.68	159.67	123.22
14	2	503	BCR	C21-C20-C19	11.66	159.62	123.22
14	3	504	BCR	C21-C20-C19	11.60	159.42	123.22
14	A	4005	BCR	C10-C11-C12	-11.59	87.05	123.22
14	4	503	BCR	C21-C20-C19	11.41	158.83	123.22
14	B	4004	BCR	C21-C20-C19	11.40	158.78	123.22
14	B	4003	BCR	C11-C12-C13	11.38	158.39	126.42
14	A	4006	BCR	C11-C12-C13	11.36	158.33	126.42
14	A	4005	BCR	C21-C20-C19	11.36	158.67	123.22
14	B	4002	BCR	C11-C10-C9	11.34	143.50	127.31
14	B	4001	BCR	C21-C20-C19	11.28	158.43	123.22
14	A	4005	BCR	C11-C12-C13	-11.11	95.22	126.42
14	B	4005	BCR	C21-C20-C19	11.09	157.82	123.22
14	B	4006	BCR	C11-C12-C13	11.06	157.49	126.42
14	A	4006	BCR	C21-C20-C19	10.83	157.00	123.22
14	3	503	BCR	C21-C20-C19	10.75	156.75	123.22
14	A	4002	BCR	C11-C12-C13	10.74	156.59	126.42
14	A	4007	BCR	C21-C20-C19	10.69	156.56	123.22
14	1	503	BCR	C21-C20-C19	10.58	156.23	123.22
14	A	4004	BCR	C11-C12-C13	10.57	156.11	126.42
14	A	4005	BCR	C35-C13-C12	10.56	134.71	118.08
14	B	4005	BCR	C11-C12-C13	10.47	155.83	126.42
14	A	4003	BCR	C21-C20-C19	10.40	155.68	123.22
14	B	4002	BCR	C11-C12-C13	10.12	154.85	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	503	BCR	C11-C12-C13	9.98	154.45	126.42
14	B	4004	BCR	C11-C12-C13	9.97	154.44	126.42
14	2	503	BCR	C11-C12-C13	9.88	154.18	126.42
14	A	4007	BCR	C11-C12-C13	9.86	154.12	126.42
14	F	4002	BCR	C11-C12-C13	9.78	153.90	126.42
15	B	1215	CLA	C4A-NA-C1A	9.72	111.08	106.71
14	4	505	BCR	C11-C12-C13	9.67	153.58	126.42
14	A	4006	BCR	C20-C19-C18	9.60	153.38	126.42
14	J	4002	BCR	C11-C12-C13	9.56	153.27	126.42
14	3	503	BCR	C11-C12-C13	9.51	153.13	126.42
15	B	1230	CLA	C4A-NA-C1A	9.45	110.95	106.71
14	1	505	BCR	C11-C12-C13	9.44	152.92	126.42
14	4	505	BCR	C20-C19-C18	9.34	152.66	126.42
15	B	1226	CLA	C4A-NA-C1A	9.28	110.88	106.71
14	3	504	BCR	C11-C12-C13	9.25	152.40	126.42
14	B	4001	BCR	C11-C12-C13	9.25	152.39	126.42
14	B	4005	BCR	C20-C19-C18	9.20	152.27	126.42
15	A	1126	CLA	C4A-NA-C1A	9.12	110.81	106.71
15	3	603	CLA	C4A-NA-C1A	9.08	110.79	106.71
15	B	1021	CLA	C4A-NA-C1A	9.07	110.78	106.71
15	2	606	CLA	C4A-NA-C1A	9.01	110.76	106.71
15	A	1106	CLA	C4A-NA-C1A	9.01	110.75	106.71
12	1	501	LUT	C31-C30-C29	-9.00	114.46	127.31
15	B	1229	CLA	C4A-NA-C1A	8.98	110.74	106.71
15	F	1301	CLA	C4A-NA-C1A	8.93	110.72	106.71
15	A	1104	CLA	C4A-NA-C1A	8.93	110.72	106.71
15	B	1205	CLA	C4A-NA-C1A	8.92	110.72	106.71
15	B	1227	CLA	C4A-NA-C1A	8.84	110.68	106.71
14	A	4004	BCR	C20-C19-C18	8.83	151.23	126.42
15	A	1127	CLA	C4A-NA-C1A	8.82	110.67	106.71
14	A	4005	BCR	C20-C19-C18	8.82	151.19	126.42
15	A	1115	CLA	C4A-NA-C1A	8.80	110.66	106.71
15	2	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
15	B	1202	CLA	C4A-NA-C1A	8.76	110.65	106.71
15	B	1206	CLA	C4A-NA-C1A	8.74	110.64	106.71
15	A	1102	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	A	1134	CLA	C4A-NA-C1A	8.73	110.63	106.71
15	B	1203	CLA	C4A-NA-C1A	8.72	110.63	106.71
15	B	1223	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	B	1221	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	3	601	CLA	C4A-NA-C1A	8.71	110.62	106.71
15	A	1129	CLA	C4A-NA-C1A	8.70	110.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	503	BCR	C20-C19-C18	8.69	150.84	126.42
15	2	605	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	1	608	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	2	602	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	2	607	CLA	C4A-NA-C1A	8.69	110.61	106.71
15	4	612	CLA	C4A-NA-C1A	8.67	110.61	106.71
14	3	504	BCR	C20-C19-C18	8.65	150.70	126.42
15	A	1128	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	A	1132	CLA	C4A-NA-C1A	8.64	110.59	106.71
15	4	608	CLA	C4A-NA-C1A	8.62	110.58	106.71
15	A	1130	CLA	C4A-NA-C1A	8.62	110.58	106.71
14	4	503	BCR	C20-C19-C18	8.59	150.56	126.42
15	B	1234	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	1	607	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	A	1118	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	4	605	CLA	C4A-NA-C1A	8.59	110.57	106.71
15	A	1131	CLA	C4A-NA-C1A	8.58	110.56	106.71
15	A	1141	CLA	C4A-NA-C1A	8.58	110.56	106.71
14	B	4003	BCR	C20-C19-C18	8.57	150.50	126.42
14	3	503	BCR	C20-C19-C18	8.57	150.50	126.42
15	A	1135	CLA	C4A-NA-C1A	8.57	110.56	106.71
15	B	1236	CLA	C4A-NA-C1A	8.57	110.56	106.71
15	B	1218	CLA	C4A-NA-C1A	8.56	110.56	106.71
15	A	1117	CLA	C4A-NA-C1A	8.56	110.56	106.71
15	A	1110	CLA	C4A-NA-C1A	8.56	110.56	106.71
14	1	505	BCR	C20-C19-C18	8.55	150.44	126.42
15	A	1116	CLA	C4A-NA-C1A	8.55	110.55	106.71
15	4	606	CLA	C4A-NA-C1A	8.54	110.55	106.71
15	A	1139	CLA	C4A-NA-C1A	8.54	110.55	106.71
15	1	615	CLA	C4A-NA-C1A	8.52	110.54	106.71
15	2	608	CLA	C4A-NA-C1A	8.52	110.54	106.71
15	B	1210	CLA	C4A-NA-C1A	8.52	110.53	106.71
12	1	501	LUT	C15-C35-C34	-8.51	106.05	123.47
15	B	1222	CLA	C4A-NA-C1A	8.46	110.51	106.71
15	A	1123	CLA	C4A-NA-C1A	8.45	110.51	106.71
14	B	4004	BCR	C20-C19-C18	8.45	150.15	126.42
15	A	1109	CLA	C4A-NA-C1A	8.45	110.50	106.71
15	1	606	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	J	1302	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	A	1114	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	B	1240	CLA	C4A-NA-C1A	8.44	110.50	106.71
15	A	1125	CLA	C4A-NA-C1A	8.44	110.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	615	CLA	C4A-NA-C1A	8.43	110.50	106.71
15	A	1108	CLA	C4A-NA-C1A	8.42	110.49	106.71
15	B	1208	CLA	C4A-NA-C1A	8.41	110.48	106.71
15	A	1105	CLA	C4A-NA-C1A	8.40	110.48	106.71
15	B	1238	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	2	503	BCR	C20-C19-C18	8.38	149.97	126.42
15	A	1120	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	1	611	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	B	1219	CLA	C4A-NA-C1A	8.38	110.47	106.71
15	A	1112	CLA	C4A-NA-C1A	8.37	110.47	106.71
15	B	1237	CLA	C4A-NA-C1A	8.37	110.47	106.71
15	2	615	CLA	C4A-NA-C1A	8.36	110.46	106.71
15	A	1121	CLA	C4A-NA-C1A	8.36	110.46	106.71
15	A	1113	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	J	4002	BCR	C20-C19-C18	8.33	149.83	126.42
14	A	4005	BCR	C12-C13-C14	-8.33	106.15	118.94
15	4	609	CLA	C4A-NA-C1A	8.33	110.45	106.71
14	J	4001	BCR	C20-C19-C18	8.33	149.81	126.42
15	A	1124	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	A	1138	CLA	C4A-NA-C1A	8.31	110.44	106.71
15	3	607	CLA	C4A-NA-C1A	8.30	110.44	106.71
15	1	613	CLA	C4A-NA-C1A	8.29	110.43	106.71
15	B	1231	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	A	1122	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	1	612	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	3	608	CLA	C4A-NA-C1A	8.26	110.42	106.71
15	A	1119	CLA	C4A-NA-C1A	8.25	110.41	106.71
15	A	1140	CLA	C4A-NA-C1A	8.24	110.41	106.71
15	1	602	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	B	1214	CLA	C4A-NA-C1A	8.23	110.41	106.71
15	B	1022	CLA	C4A-NA-C1A	8.23	110.40	106.71
15	B	1201	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	B	1212	CLA	C4A-NA-C1A	8.22	110.40	106.71
15	3	613	CLA	C4A-NA-C1A	8.21	110.40	106.71
15	A	1013	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	B	1209	CLA	C4A-NA-C1A	8.20	110.39	106.71
15	3	606	CLA	C4A-NA-C1A	8.19	110.39	106.71
15	3	612	CLA	C4A-NA-C1A	8.19	110.39	106.71
15	A	1101	CLA	C4A-NA-C1A	8.18	110.38	106.71
15	1	603	CLA	C4A-NA-C1A	8.16	110.37	106.71
15	B	1220	CLA	C4A-NA-C1A	8.15	110.37	106.71
15	3	611	CLA	C4A-NA-C1A	8.13	110.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1107	CLA	C4A-NA-C1A	8.12	110.36	106.71
14	B	4006	BCR	C20-C19-C18	8.12	149.22	126.42
15	B	1239	CLA	C4A-NA-C1A	8.11	110.35	106.71
15	B	1232	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	A	1111	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	B	1217	CLA	C4A-NA-C1A	8.10	110.35	106.71
15	1	601	CLA	C4A-NA-C1A	8.09	110.34	106.71
14	A	4005	BCR	C11-C10-C9	8.08	138.84	127.31
14	B	4002	BCR	C20-C19-C18	8.08	149.11	126.42
15	4	615	CLA	C4A-NA-C1A	8.08	110.34	106.71
15	B	1023	CLA	C4A-NA-C1A	8.06	110.33	106.71
15	B	1224	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	J	4003	BCR	C20-C19-C18	8.06	149.05	126.42
15	B	1211	CLA	C4A-NA-C1A	8.05	110.33	106.71
15	B	1225	CLA	C4A-NA-C1A	8.03	110.31	106.71
15	B	1216	CLA	C4A-NA-C1A	8.02	110.31	106.71
15	A	1136	CLA	C4A-NA-C1A	8.01	110.31	106.71
15	A	1137	CLA	C4A-NA-C1A	8.00	110.30	106.71
15	3	605	CLA	C4A-NA-C1A	7.99	110.30	106.71
15	F	1302	CLA	C4A-NA-C1A	7.98	110.29	106.71
15	1	605	CLA	C4A-NA-C1A	7.95	110.28	106.71
15	4	602	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	2	603	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	A	1133	CLA	C4A-NA-C1A	7.92	110.27	106.71
15	4	603	CLA	C4A-NA-C1A	7.91	110.26	106.71
15	A	1012	CLA	C4A-NA-C1A	7.90	110.26	106.71
14	F	4002	BCR	C20-C19-C18	7.90	148.60	126.42
15	3	610	CLA	C4A-NA-C1A	7.87	110.24	106.71
15	B	1204	CLA	C4A-NA-C1A	7.85	110.24	106.71
15	4	604	CLA	C4A-NA-C1A	7.85	110.23	106.71
15	1	604	CLA	C4A-NA-C1A	7.84	110.23	106.71
14	B	4001	BCR	C20-C19-C18	7.78	148.27	126.42
15	A	1103	CLA	C4A-NA-C1A	7.77	110.20	106.71
15	4	601	CLA	C4A-NA-C1A	7.72	110.18	106.71
15	2	601	CLA	C4A-NA-C1A	7.70	110.17	106.71
15	B	1235	CLA	C4A-NA-C1A	7.52	110.09	106.71
12	1	501	LUT	C37-C21-C26	7.51	120.92	109.55
15	B	1228	CLA	C4A-NA-C1A	7.41	110.04	106.71
15	B	1213	CLA	C4A-NA-C1A	7.28	109.98	106.71
14	A	4005	BCR	C8-C9-C10	-7.27	107.79	118.94
15	2	604	CLA	C4A-NA-C1A	7.18	109.93	106.71
15	4	607	CLA	C4A-NA-C1A	7.16	109.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4002	BCR	C20-C19-C18	7.02	146.12	126.42
14	A	4007	BCR	C20-C19-C18	6.73	145.31	126.42
15	B	1207	CLA	C2A-C1A-CHA	-6.68	111.23	122.63
14	A	4007	BCR	C15-C14-C13	-6.60	117.89	127.31
14	A	4003	BCR	C20-C19-C18	6.55	144.81	126.42
15	3	603	CLA	O2D-CGD-CBD	6.52	122.86	111.27
24	A	1011	CL0	C4A-NA-C1A	6.44	109.60	106.71
24	A	1011	CL0	C2C-C1C-NC	6.28	115.86	109.97
12	4	501	LUT	C21-C26-C25	6.16	122.45	111.42
12	1	501	LUT	C21-C26-C27	6.03	120.33	112.70
15	A	1111	CLA	O2D-CGD-CBD	5.94	121.81	111.27
15	B	1211	CLA	O2A-C1-C2	5.93	122.83	108.97
15	4	609	CLA	O2A-C1-C2	5.87	122.71	108.97
15	3	601	CLA	O2A-C1-C2	5.87	122.69	108.97
15	2	608	CLA	O2A-C1-C2	5.81	122.56	108.97
13	1	502	XAT	C31-C30-C29	-5.79	119.05	127.31
15	1	606	CLA	O2D-CGD-CBD	5.79	121.55	111.27
15	A	1101	CLA	O2D-CGD-CBD	5.79	121.55	111.27
15	A	1109	CLA	O2A-C1-C2	5.77	122.46	108.97
15	4	605	CLA	O2D-CGD-CBD	5.75	121.49	111.27
15	4	602	CLA	O2A-C1-C2	5.75	122.42	108.97
12	3	501	LUT	C21-C26-C25	5.74	121.70	111.42
14	B	4001	BCR	C15-C14-C13	-5.73	119.13	127.31
15	A	1124	CLA	O2A-C1-C2	5.72	122.33	108.97
15	4	609	CLA	O2D-CGD-CBD	5.71	121.42	111.27
15	A	1110	CLA	O2A-C1-C2	5.71	122.32	108.97
15	B	1215	CLA	O2D-CGD-CBD	5.68	121.37	111.27
15	A	1107	CLA	O2A-C1-C2	5.65	122.18	108.97
15	1	604	CLA	O2D-CGD-CBD	5.64	121.30	111.27
15	1	604	CLA	O2A-C1-C2	5.64	122.16	108.97
15	4	603	CLA	O2A-C1-C2	5.64	122.15	108.97
12	2	501	LUT	C15-C14-C13	-5.62	119.28	127.31
15	3	601	CLA	O2D-CGD-CBD	5.61	121.24	111.27
15	A	1111	CLA	O2A-C1-C2	5.60	122.08	108.97
15	B	1226	CLA	O2D-CGD-CBD	5.59	121.20	111.27
15	A	1137	CLA	O2D-CGD-CBD	5.59	121.19	111.27
15	4	601	CLA	O2A-C1-C2	5.58	122.03	108.97
15	B	1236	CLA	O2D-CGD-CBD	5.58	121.18	111.27
15	2	604	CLA	O2D-CGD-CBD	5.58	121.18	111.27
12	2	501	LUT	C11-C10-C9	-5.58	119.35	127.31
15	1	608	CLA	O2D-CGD-CBD	5.58	121.18	111.27
15	4	606	CLA	O2A-C1-C2	5.57	122.00	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1205	CLA	O2A-C1-C2	5.57	122.00	108.97
15	4	604	CLA	O2D-CGD-CBD	5.57	121.17	111.27
15	A	1132	CLA	O2D-CGD-CBD	5.53	121.10	111.27
15	1	601	CLA	O2A-C1-C2	5.53	121.89	108.97
15	A	1137	CLA	O2A-C1-C2	5.52	121.89	108.97
15	B	1225	CLA	O2A-C1-C2	5.52	121.87	108.97
15	B	1230	CLA	O2A-C1-C2	5.51	121.86	108.97
15	B	1222	CLA	O2D-CGD-CBD	5.51	121.07	111.27
15	B	1232	CLA	O2A-C1-C2	5.51	121.86	108.97
15	B	1224	CLA	O2A-C1-C2	5.50	121.83	108.97
15	A	1118	CLA	O2A-C1-C2	5.50	121.82	108.97
15	1	615	CLA	O2D-CGD-CBD	5.50	121.03	111.27
15	B	1208	CLA	O2A-C1-C2	5.49	121.81	108.97
12	1	501	LUT	C32-C33-C34	5.49	127.36	118.94
15	A	1104	CLA	O2D-CGD-CBD	5.48	121.00	111.27
15	A	1128	CLA	O2D-CGD-CBD	5.48	121.00	111.27
13	4	502	XAT	C31-C30-C29	-5.48	119.49	127.31
12	1	501	LUT	C31-C32-C33	-5.48	111.03	126.42
15	3	612	CLA	O2D-CGD-CBD	5.47	120.99	111.27
15	A	1119	CLA	O2A-C1-C2	5.47	121.75	108.97
15	B	1222	CLA	O2A-C1-C2	5.47	121.75	108.97
15	A	1115	CLA	O2D-CGD-CBD	5.45	120.95	111.27
15	2	601	CLA	O2A-C1-C2	5.45	121.70	108.97
15	B	1235	CLA	O2D-CGD-CBD	5.44	120.93	111.27
15	A	1125	CLA	O2A-C1-C2	5.44	121.68	108.97
15	B	1223	CLA	O2D-CGD-CBD	5.42	120.90	111.27
15	B	1218	CLA	O2A-C1-C2	5.42	121.64	108.97
15	B	1205	CLA	O2D-CGD-CBD	5.42	120.89	111.27
15	B	1234	CLA	O2A-C1-C2	5.41	121.63	108.97
15	A	1102	CLA	O2D-CGD-CBD	5.41	120.88	111.27
15	A	1127	CLA	O2A-C1-C2	5.41	121.62	108.97
15	A	1122	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1112	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1117	CLA	O2A-C1-C2	5.40	121.59	108.97
15	A	1134	CLA	O2A-C1-C2	5.39	121.58	108.97
15	A	1135	CLA	O2A-C1-C2	5.39	121.58	108.97
15	B	1210	CLA	O2A-C1-C2	5.39	121.58	108.97
15	1	611	CLA	O2A-C1-C2	5.39	121.57	108.97
15	1	605	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	A	1011	CL0	C1-C2-C3	-5.38	118.05	126.75
15	B	1215	CLA	O2A-C1-C2	5.38	121.54	108.97
15	4	612	CLA	O2D-CGD-CBD	5.38	120.82	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1120	CLA	O2A-C1-C2	5.38	121.54	108.97
12	1	501	LUT	C37-C21-C22	5.37	119.60	109.44
15	A	1140	CLA	O2D-CGD-CBD	5.37	120.81	111.27
15	B	1214	CLA	O2A-C1-C2	5.36	121.52	108.97
15	2	607	CLA	O2A-C1-C2	5.35	121.49	108.97
15	B	1206	CLA	O2A-C1-C2	5.35	121.48	108.97
15	2	602	CLA	O2A-C1-C2	5.35	121.48	108.97
15	2	612	CLA	O2A-C1-C2	5.35	121.47	108.97
15	4	612	CLA	O2A-C1-C2	5.34	121.46	108.97
15	B	1204	CLA	O2D-CGD-CBD	5.34	120.76	111.27
15	4	604	CLA	O2A-C1-C2	5.33	121.44	108.97
14	3	504	BCR	C15-C14-C13	-5.33	119.70	127.31
15	B	1221	CLA	O2D-CGD-CBD	5.33	120.75	111.27
15	A	1108	CLA	O2D-CGD-CBD	5.33	120.75	111.27
14	J	4002	BCR	C15-C14-C13	-5.33	119.70	127.31
14	A	4005	BCR	C34-C9-C10	5.33	130.39	122.92
15	A	1105	CLA	O2A-C1-C2	5.33	121.43	108.97
15	A	1134	CLA	O2D-CGD-CBD	5.33	120.74	111.27
12	2	501	LUT	C21-C26-C27	5.33	119.44	112.70
15	A	1103	CLA	O2D-CGD-CBD	5.32	120.72	111.27
15	A	1116	CLA	O2A-C1-C2	5.32	121.41	108.97
24	A	1011	CL0	C1C-C2C-C3C	-5.32	101.37	106.96
15	A	1128	CLA	O2A-C1-C2	5.31	121.39	108.97
12	1	501	LUT	C35-C15-C14	5.31	134.35	123.47
13	1	502	XAT	C7-C8-C9	-5.30	117.31	125.53
15	B	1216	CLA	O2A-C1-C2	5.29	121.35	108.97
15	B	1213	CLA	O2A-C1-C2	5.29	121.33	108.97
15	B	1021	CLA	O2A-C1-C2	5.28	122.52	108.64
15	3	606	CLA	O2D-CGD-CBD	5.28	120.65	111.27
15	B	1220	CLA	O2A-C1-C2	5.27	122.49	108.64
15	B	1216	CLA	O2D-CGD-CBD	5.27	120.64	111.27
15	1	602	CLA	O2D-CGD-CBD	5.26	120.62	111.27
15	A	1114	CLA	O2D-CGD-CBD	5.26	120.61	111.27
15	A	1136	CLA	O2A-C1-C2	5.26	121.26	108.97
15	A	1115	CLA	O2A-C1-C2	5.25	121.24	108.97
15	B	1225	CLA	O2D-CGD-CBD	5.24	120.58	111.27
15	B	1236	CLA	O2A-C1-C2	5.24	121.22	108.97
12	2	501	LUT	C21-C26-C25	5.24	120.80	111.42
15	B	1202	CLA	O2A-C1-C2	5.24	121.22	108.97
15	A	1133	CLA	O2A-C1-C2	5.23	121.19	108.97
15	B	1212	CLA	O2D-CGD-CBD	5.22	120.54	111.27
15	4	607	CLA	O2D-CGD-CBD	5.21	120.53	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	612	CLA	O2D-CGD-CBD	5.21	120.53	111.27
15	B	1213	CLA	O2D-CGD-CBD	5.20	120.51	111.27
15	B	1214	CLA	O2D-CGD-CBD	5.20	120.50	111.27
15	A	1136	CLA	O2D-CGD-CBD	5.20	120.50	111.27
15	B	1022	CLA	O2A-C1-C2	5.20	122.29	108.64
15	B	1237	CLA	O2A-C1-C2	5.19	121.11	108.97
15	A	1132	CLA	O2A-C1-C2	5.19	121.10	108.97
15	A	1126	CLA	O2A-C1-C2	5.18	121.07	108.97
15	A	1105	CLA	O2D-CGD-CBD	5.17	120.46	111.27
15	B	1239	CLA	O2A-C1-C2	5.17	122.23	108.64
15	B	1227	CLA	O2D-CGD-CBD	5.17	120.46	111.27
15	B	1226	CLA	O2A-C1-C2	5.17	121.06	108.97
15	B	1220	CLA	O2D-CGD-CBD	5.16	120.44	111.27
15	B	1240	CLA	O2A-C1-C2	5.16	122.19	108.64
15	B	1219	CLA	O2A-C1-C2	5.15	121.01	108.97
15	3	610	CLA	O2A-C1-C2	5.15	121.01	108.97
12	1	501	LUT	C12-C13-C14	-5.12	111.08	118.94
15	2	606	CLA	O2D-CGD-CBD	5.12	120.37	111.27
14	J	4003	BCR	C33-C5-C6	-5.12	118.78	124.53
15	1	613	CLA	O2D-CGD-CBD	5.12	120.36	111.27
15	A	1106	CLA	O2D-CGD-CBD	5.12	120.36	111.27
13	2	502	XAT	C15-C14-C13	-5.11	120.01	127.31
15	4	607	CLA	O2A-C1-C2	5.11	120.92	108.97
15	A	1121	CLA	O2A-C1-C2	5.11	120.91	108.97
15	B	1221	CLA	O2A-C1-C2	5.11	120.91	108.97
15	2	602	CLA	O2D-CGD-CBD	5.10	120.33	111.27
15	B	1235	CLA	O2A-C1-C2	5.10	122.04	108.64
13	2	502	XAT	C38-C25-C24	5.10	120.01	114.28
15	2	608	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1209	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1210	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1229	CLA	O2D-CGD-CBD	5.08	120.29	111.27
15	B	1203	CLA	O2A-C1-C2	5.07	120.83	108.97
15	1	612	CLA	O2A-C1-C2	5.07	121.95	108.64
15	2	607	CLA	O2D-CGD-CBD	5.06	120.26	111.27
15	A	1131	CLA	O2D-CGD-CBD	5.05	120.25	111.27
15	A	1012	CLA	O2A-C1-C2	5.05	121.91	108.64
13	3	502	XAT	C31-C30-C29	-5.05	120.10	127.31
15	B	1237	CLA	O2D-CGD-CBD	5.05	120.24	111.27
15	4	605	CLA	O2A-C1-C2	5.05	120.77	108.97
15	A	1141	CLA	O2D-CGD-CBD	5.04	120.23	111.27
15	A	1122	CLA	O2D-CGD-CBD	5.04	120.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	602	CLA	O2D-CGD-CBD	5.04	120.22	111.27
15	B	1239	CLA	O2D-CGD-CBD	5.04	120.22	111.27
15	A	1126	CLA	O2D-CGD-CBD	5.03	120.21	111.27
15	B	1201	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	B	1231	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	A	1109	CLA	O2D-CGD-CBD	5.03	120.20	111.27
15	A	1116	CLA	O2D-CGD-CBD	5.02	120.19	111.27
15	B	1238	CLA	O2D-CGD-CBD	5.02	120.19	111.27
15	1	603	CLA	O2D-CGD-CBD	5.02	120.19	111.27
13	1	502	XAT	C15-C14-C13	-5.02	120.14	127.31
14	A	4007	BCR	C33-C5-C6	-5.01	118.90	124.53
15	A	1130	CLA	O2A-C1-C2	5.01	121.79	108.64
13	4	502	XAT	C15-C14-C13	-5.01	120.17	127.31
18	1	803	LMG	O7-C10-C11	5.00	120.29	111.09
15	A	1127	CLA	O2D-CGD-CBD	5.00	120.16	111.27
15	1	611	CLA	O2D-CGD-CBD	5.00	120.15	111.27
15	A	1130	CLA	O2D-CGD-CBD	4.99	120.13	111.27
15	A	1120	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	2	603	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	B	1022	CLA	O2D-CGD-CBD	4.98	120.12	111.27
15	A	1124	CLA	O2D-CGD-CBD	4.98	120.11	111.27
15	A	1121	CLA	O2D-CGD-CBD	4.97	120.11	111.27
15	4	615	CLA	O2A-C1-C2	4.97	121.69	108.64
15	F	1301	CLA	O2D-CGD-CBD	4.97	120.09	111.27
15	B	1204	CLA	O2A-C1-C2	4.96	120.57	108.97
15	4	608	CLA	O2D-CGD-CBD	4.96	120.08	111.27
15	A	1104	CLA	O2A-C1-C2	4.95	121.66	108.64
15	2	604	CLA	O2A-C1-C2	4.95	120.55	108.97
15	A	1123	CLA	O2D-CGD-CBD	4.95	120.06	111.27
15	2	615	CLA	O2A-C1-C2	4.94	121.63	108.64
13	1	502	XAT	C18-C5-C4	4.94	119.84	114.28
15	2	615	CLA	O2D-CGD-CBD	4.94	120.04	111.27
15	A	1113	CLA	O2D-CGD-CBD	4.93	120.03	111.27
15	B	1232	CLA	O2D-CGD-CBD	4.93	120.03	111.27
15	A	1106	CLA	O2A-C1-C2	4.93	121.58	108.64
15	3	607	CLA	O2D-CGD-CBD	4.92	120.00	111.27
15	F	1302	CLA	O2A-C1-C2	4.90	120.44	108.97
15	A	1129	CLA	O2D-CGD-CBD	4.89	119.96	111.27
15	3	615	CLA	O2D-CGD-CBD	4.89	119.95	111.27
15	3	608	CLA	O2D-CGD-CBD	4.89	119.95	111.27
15	B	1223	CLA	O2A-C1-C2	4.88	121.47	108.64
15	B	1228	CLA	O2A-C1-C2	4.88	121.46	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1135	CLA	O2D-CGD-CBD	4.88	119.93	111.27
15	B	1211	CLA	O2D-CGD-CBD	4.88	119.93	111.27
15	A	1112	CLA	O2D-CGD-CBD	4.87	119.92	111.27
13	3	502	XAT	C7-C8-C9	-4.87	117.98	125.53
15	2	605	CLA	O2D-CGD-CBD	4.86	119.90	111.27
17	2	801	LHG	O7-C7-C8	4.86	120.03	111.09
17	B	5001	LHG	O7-C7-C8	4.86	120.03	111.09
15	A	1133	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	A	1139	CLA	O2D-CGD-CBD	4.85	119.89	111.27
15	A	1117	CLA	O2D-CGD-CBD	4.85	119.88	111.27
14	J	4001	BCR	C33-C5-C6	-4.85	119.09	124.53
15	A	1118	CLA	O2D-CGD-CBD	4.85	119.88	111.27
15	A	1107	CLA	O2D-CGD-CBD	4.84	119.88	111.27
15	B	1228	CLA	O2D-CGD-CBD	4.84	119.88	111.27
15	2	605	CLA	O2A-C1-C2	4.84	121.34	108.64
15	A	1012	CLA	O2D-CGD-CBD	4.83	119.85	111.27
15	B	1234	CLA	O2D-CGD-CBD	4.83	119.84	111.27
14	F	4002	BCR	C15-C14-C13	-4.82	120.43	127.31
15	4	606	CLA	O2D-CGD-CBD	4.82	119.83	111.27
15	A	1119	CLA	O2D-CGD-CBD	4.81	119.82	111.27
15	3	613	CLA	O2D-CGD-CBD	4.81	119.81	111.27
13	2	502	XAT	C31-C30-C29	-4.80	120.46	127.31
15	3	612	CLA	O2A-C1-C2	4.80	121.25	108.64
12	1	501	LUT	C15-C14-C13	4.79	134.14	127.31
15	J	1302	CLA	O2A-C1-C2	4.79	120.17	108.97
15	A	1139	CLA	O2A-C1-C2	4.78	121.21	108.64
15	F	1302	CLA	O2D-CGD-CBD	4.77	119.75	111.27
15	B	1023	CLA	O2A-C1-C2	4.77	121.18	108.64
13	4	502	XAT	C38-C25-C24	4.77	119.65	114.28
15	A	1138	CLA	O2A-C1-C2	4.77	121.17	108.64
15	B	1230	CLA	O2D-CGD-CBD	4.76	119.72	111.27
15	B	1219	CLA	O2D-CGD-CBD	4.75	119.71	111.27
15	1	607	CLA	O2D-CGD-CBD	4.75	119.71	111.27
15	A	1103	CLA	O2A-C1-C2	4.75	121.11	108.64
15	B	1208	CLA	O2D-CGD-CBD	4.74	119.69	111.27
24	A	1011	CL0	O2A-CGA-O1A	-4.71	111.70	123.59
15	J	1302	CLA	O2D-CGD-CBD	4.71	119.64	111.27
15	A	1138	CLA	O2D-CGD-CBD	4.71	119.63	111.27
15	B	1224	CLA	O2D-CGD-CBD	4.70	119.62	111.27
15	B	1217	CLA	O2D-CGD-CBD	4.70	119.62	111.27
15	A	1141	CLA	O2A-C1-C2	4.69	120.97	108.64
15	3	610	CLA	O2D-CGD-CBD	4.69	119.60	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	501	LUT	C40-C33-C34	-4.68	116.36	122.92
15	1	615	CLA	O2A-C1-C2	4.67	120.91	108.64
15	A	1140	CLA	O2A-C1-C2	4.66	120.89	108.64
15	3	607	CLA	O2A-C1-C2	4.66	120.89	108.64
15	B	1206	CLA	O2D-CGD-CBD	4.66	119.55	111.27
15	A	1125	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	A	1011	CL0	O2A-C1-C2	4.63	120.81	108.64
15	3	611	CLA	O2D-CGD-CBD	4.63	119.50	111.27
15	B	1238	CLA	O2A-C1-C2	4.63	120.80	108.64
15	B	1218	CLA	O2D-CGD-CBD	4.63	119.49	111.27
15	B	1202	CLA	O2D-CGD-CBD	4.63	119.49	111.27
12	1	501	LUT	C18-C5-C6	-4.63	119.33	124.53
12	3	501	LUT	C11-C10-C9	-4.62	120.71	127.31
15	B	1203	CLA	O2D-CGD-CBD	4.61	119.47	111.27
14	F	4002	BCR	C33-C5-C6	-4.61	119.35	124.53
15	A	1131	CLA	O2A-C1-C2	4.61	120.74	108.64
15	A	1013	CLA	O2D-CGD-CBD	4.61	119.45	111.27
12	1	501	LUT	C21-C26-C25	4.60	119.67	111.42
15	B	1231	CLA	O2A-C1-C2	4.57	120.64	108.64
12	3	501	LUT	C18-C5-C6	-4.57	119.40	124.53
13	2	502	XAT	C18-C5-C4	4.56	119.42	114.28
14	2	503	BCR	C33-C5-C6	-4.55	119.42	124.53
15	4	603	CLA	O2D-CGD-CBD	4.54	119.34	111.27
15	B	1021	CLA	O2D-CGD-CBD	4.54	119.34	111.27
15	4	601	CLA	O2D-CGD-CBD	4.52	119.30	111.27
17	A	5002	LHG	O7-C7-C8	4.51	121.22	111.50
12	3	501	LUT	C7-C8-C9	-4.49	119.44	126.23
14	B	4004	BCR	C33-C5-C6	-4.48	119.49	124.53
18	1	802	LMG	O7-C10-C11	4.47	121.14	111.50
15	3	605	CLA	O2D-CGD-CBD	4.47	119.21	111.27
14	B	4002	BCR	C15-C14-C13	-4.47	120.93	127.31
14	J	4002	BCR	C4-C5-C6	-4.46	116.25	122.73
12	3	501	LUT	C21-C26-C27	4.46	118.34	112.70
13	3	502	XAT	C18-C5-C4	4.45	119.29	114.28
12	4	501	LUT	C18-C5-C6	-4.45	119.53	124.53
14	A	4004	BCR	C33-C5-C6	-4.44	119.54	124.53
15	B	1207	CLA	C2D-C3D-C4D	-4.44	102.48	106.30
14	B	4005	BCR	C33-C5-C6	-4.43	119.55	124.53
15	1	601	CLA	O2D-CGD-CBD	4.41	119.10	111.27
13	4	502	XAT	C18-C5-C4	4.39	119.22	114.28
15	1	612	CLA	C1-C2-C3	-4.39	118.45	126.04
13	1	502	XAT	C38-C25-C24	4.38	119.21	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1110	CLA	O2D-CGD-CBD	4.34	118.98	111.27
24	A	1011	CL0	O2D-CGD-CBD	4.34	118.98	111.27
14	3	504	BCR	C33-C5-C6	-4.34	119.66	124.53
13	3	502	XAT	C38-C25-C24	4.31	119.13	114.28
14	A	4002	BCR	C33-C5-C6	-4.29	119.71	124.53
15	B	1207	CLA	C1C-NC-C4C	4.29	108.64	106.71
15	B	1229	CLA	O2A-C1-C2	4.28	119.89	108.64
12	2	501	LUT	C7-C8-C9	-4.28	119.77	126.23
14	1	505	BCR	C33-C5-C6	-4.28	119.72	124.53
12	2	501	LUT	C18-C5-C6	-4.26	119.74	124.53
14	B	4002	BCR	C33-C5-C6	-4.24	119.76	124.53
17	1	801	LHG	O7-C7-C8	4.23	120.62	111.50
12	3	501	LUT	C35-C34-C33	-4.22	121.29	127.31
14	4	503	BCR	C33-C5-C6	-4.20	119.81	124.53
12	1	501	LUT	C20-C13-C12	4.18	124.66	118.08
15	1	612	CLA	O2D-CGD-CBD	4.18	118.69	111.27
15	A	1013	CLA	O2A-C1-C2	4.15	119.55	108.64
15	B	1223	CLA	C1-C2-C3	-4.15	120.05	126.75
21	2	811	DGD	O2G-C1B-C2B	4.13	120.39	111.50
15	4	615	CLA	O2D-CGD-CBD	4.12	118.59	111.27
15	B	1240	CLA	O2D-CGD-CBD	4.10	118.56	111.27
14	J	4002	BCR	C33-C5-C4	4.10	121.50	113.62
23	4	831	GSH	CA2-CB2-SG2	-4.10	109.58	114.19
14	B	4003	BCR	C33-C5-C6	-4.09	119.94	124.53
12	1	501	LUT	C10-C11-C12	-4.08	110.47	123.22
23	B	5031	GSH	CA2-CB2-SG2	-4.07	109.62	114.19
15	2	601	CLA	O2D-CGD-CBD	4.02	118.42	111.27
15	4	615	CLA	C1-C2-C3	-4.02	119.09	126.04
14	A	4006	BCR	C33-C5-C6	-4.02	120.01	124.53
15	B	1023	CLA	O2D-CGD-CBD	4.00	118.37	111.27
21	4	811	DGD	O2G-C1B-C2B	3.99	120.09	111.50
12	4	501	LUT	C15-C14-C13	-3.96	121.66	127.31
15	B	1022	CLA	C1-C2-C3	-3.95	120.36	126.75
14	J	4002	BCR	C1-C6-C5	-3.94	117.06	122.61
14	A	4005	BCR	C15-C14-C13	-3.94	121.69	127.31
14	3	503	BCR	C33-C5-C6	-3.92	120.13	124.53
12	4	501	LUT	C22-C23-C24	-3.91	107.29	111.74
14	2	503	BCR	C15-C14-C13	-3.88	121.77	127.31
21	B	5002	DGD	O2G-C1B-C2B	3.88	119.85	111.50
14	A	4003	BCR	C33-C5-C6	-3.87	120.18	124.53
15	A	1141	CLA	C1-C2-C3	-3.87	120.49	126.75
14	B	4001	BCR	C33-C5-C4	3.86	121.03	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	501	LUT	C15-C14-C13	-3.83	121.84	127.31
15	B	1238	CLA	C1-C2-C3	-3.82	120.56	126.75
14	1	503	BCR	C33-C5-C6	-3.79	120.27	124.53
15	B	1207	CLA	C3B-C4B-NB	3.78	113.42	110.11
14	2	503	BCR	C33-C5-C4	3.77	120.86	113.62
15	A	1012	CLA	C1-C2-C3	-3.75	119.55	126.04
15	B	1207	CLA	C3D-C2D-C1D	-3.75	103.07	106.30
12	1	501	LUT	C35-C34-C33	3.74	132.65	127.31
15	1	605	CLA	O2A-C1-C2	3.73	122.11	109.49
14	4	503	BCR	C15-C14-C13	-3.73	121.98	127.31
15	B	1021	CLA	C1-C2-C3	-3.73	119.59	126.04
15	3	603	CLA	CAC-C3C-C4C	3.73	129.65	124.81
15	A	1131	CLA	C1-C2-C3	-3.71	120.74	126.75
13	2	502	XAT	C7-C8-C9	-3.69	119.80	125.53
14	3	503	BCR	C33-C5-C4	3.69	120.70	113.62
15	3	607	CLA	C1-C2-C3	-3.68	120.80	126.75
15	A	1126	CLA	C2C-C1C-NC	3.68	113.42	109.97
24	A	1011	CL0	C4D-C3D-CAD	3.68	110.52	108.47
25	B	2002	PQN	C11-C12-C13	-3.67	120.68	126.79
14	1	503	BCR	C33-C5-C4	3.64	120.61	113.62
14	B	4004	BCR	C15-C14-C13	-3.63	122.13	127.31
14	4	505	BCR	C33-C5-C4	3.63	120.58	113.62
15	B	1235	CLA	C1-C2-C3	-3.61	119.80	126.04
17	A	5002	LHG	O8-C23-C24	3.61	120.84	111.38
15	B	1207	CLA	C4A-NA-C1A	-3.61	105.08	106.71
15	2	605	CLA	C1-C2-C3	-3.59	119.84	126.04
15	F	1301	CLA	O2A-C1-C2	3.58	121.58	108.42
16	4	610	CHL	C3C-C4C-NC	-3.58	106.56	110.57
14	A	4002	BCR	C34-C9-C10	-3.57	117.92	122.92
15	B	1201	CLA	O2A-C1-C2	3.57	121.56	109.49
15	2	615	CLA	C1-C2-C3	-3.57	120.98	126.75
13	2	502	XAT	O24-C25-C24	3.57	116.06	113.38
15	B	1228	CLA	C1-C2-C3	-3.55	119.91	126.04
15	3	615	CLA	C2C-C1C-NC	3.54	113.29	109.97
15	A	1138	CLA	C1-C2-C3	-3.54	119.92	126.04
14	J	4002	BCR	C34-C9-C10	-3.50	118.01	122.92
15	A	1104	CLA	C1-C2-C3	-3.50	119.99	126.04
14	B	4006	BCR	C33-C5-C6	-3.50	120.60	124.53
15	3	603	CLA	C2C-C1C-NC	3.50	113.25	109.97
18	2	802	LMG	O8-C28-C29	3.49	120.53	111.38
24	A	1011	CL0	O2A-CGA-CBA	3.49	122.86	111.91
15	A	1123	CLA	O2A-C1-C2	3.49	121.29	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1129	CLA	O2A-C1-C2	3.48	121.24	109.49
15	A	1012	CLA	OBD-CAD-CBD	-3.46	120.95	125.89
15	A	1130	CLA	C1-C2-C3	-3.45	120.07	126.04
14	A	4005	BCR	C33-C5-C4	3.44	120.23	113.62
14	B	4003	BCR	C33-C5-C4	3.43	120.21	113.62
25	A	2001	PQN	C11-C12-C13	-3.43	121.08	126.79
16	1	610	CHL	C1B-CHB-C4A	-3.43	123.33	130.12
15	2	606	CLA	C2C-C1C-NC	3.42	113.18	109.97
14	A	4005	BCR	C33-C5-C6	-3.41	120.70	124.53
13	4	502	XAT	C7-C8-C9	-3.41	120.24	125.53
15	4	609	CLA	C2C-C1C-NC	3.41	113.17	109.97
15	B	1223	CLA	C2C-C1C-NC	3.41	113.16	109.97
14	B	4006	BCR	C27-C26-C25	-3.40	117.79	122.73
15	2	604	CLA	C2C-C1C-NC	3.40	113.16	109.97
15	3	608	CLA	O2A-C1-C2	3.39	120.97	109.49
16	2	613	CHL	C3C-C4C-NC	-3.39	106.77	110.57
14	4	505	BCR	C33-C5-C6	-3.38	120.73	124.53
13	2	502	XAT	O4-C5-C4	-3.38	110.84	113.38
15	A	1139	CLA	C1-C2-C3	-3.38	120.19	126.04
15	B	1231	CLA	C1-C2-C3	-3.38	120.20	126.04
14	A	4005	BCR	C27-C26-C25	-3.38	117.83	122.73
15	A	1103	CLA	C2C-C1C-NC	3.38	113.13	109.97
16	3	604	CHL	C3C-C4C-NC	-3.37	106.79	110.57
16	4	613	CHL	CMA-C3A-C4A	3.37	120.83	111.77
14	B	4001	BCR	C33-C5-C6	-3.37	120.74	124.53
16	4	613	CHL	C2C-C3C-C4C	3.37	108.89	106.49
14	B	4002	BCR	C33-C5-C4	3.36	120.08	113.62
15	A	1140	CLA	C1-C2-C3	-3.36	120.24	126.04
14	A	4003	BCR	C36-C18-C17	-3.35	118.23	122.92
15	F	1301	CLA	C2C-C1C-NC	3.35	113.11	109.97
12	2	501	LUT	C35-C34-C33	-3.33	122.55	127.31
15	B	1207	CLA	C2B-C3B-C4B	-3.33	103.44	106.29
17	2	801	LHG	C5-O7-C7	-3.32	111.71	117.90
16	1	609	CHL	CMA-C3A-C4A	3.32	120.70	111.77
14	B	4005	BCR	C33-C5-C4	3.31	119.98	113.62
15	1	608	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
15	3	612	CLA	C1-C2-C3	-3.31	120.32	126.04
15	B	1221	CLA	C2C-C1C-NC	3.30	113.07	109.97
14	A	4004	BCR	C15-C14-C13	-3.30	122.59	127.31
15	3	611	CLA	C2C-C1C-NC	3.30	113.07	109.97
15	A	1012	CLA	OBD-CAD-C3D	-3.30	122.50	127.98
13	2	502	XAT	C26-C27-C28	-3.30	119.02	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1202	CLA	C2C-C1C-NC	3.29	113.06	109.97
15	1	615	CLA	C2C-C1C-NC	3.29	113.05	109.97
18	1	803	LMG	C8-O7-C10	-3.29	111.77	117.90
12	4	501	LUT	C35-C34-C33	-3.29	122.62	127.31
14	1	505	BCR	C33-C5-C4	3.29	119.93	113.62
19	1	811	SQD	O7-S-C6	-3.28	103.04	106.94
16	2	613	CHL	C2C-C3C-C4C	3.28	108.82	106.49
14	A	4002	BCR	C27-C26-C25	-3.27	117.98	122.73
15	B	1211	CLA	C2C-C1C-NC	3.27	113.04	109.97
15	A	1112	CLA	C2C-C1C-NC	3.27	113.03	109.97
18	2	802	LMG	O7-C10-C11	3.27	119.91	110.80
14	J	4002	BCR	C8-C9-C10	3.26	123.95	118.94
15	A	1135	CLA	C2C-C1C-NC	3.26	113.03	109.97
14	B	4001	BCR	C27-C26-C25	-3.26	117.99	122.73
16	1	610	CHL	CMA-C3A-C4A	3.26	120.54	111.77
14	J	4001	BCR	C27-C26-C25	-3.26	118.00	122.73
15	A	1127	CLA	C2C-C1C-NC	3.26	113.02	109.97
15	A	1104	CLA	C2C-C1C-NC	3.25	113.02	109.97
15	A	1136	CLA	C2C-C1C-NC	3.25	113.02	109.97
15	4	608	CLA	C2C-C1C-NC	3.24	113.01	109.97
16	4	613	CHL	C4A-NA-C1A	3.24	108.16	106.71
15	1	613	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	2	821	LMT	C1'-O5'-C5'	-3.23	107.56	113.66
15	A	1115	CLA	C2C-C1C-NC	3.23	113.00	109.97
14	4	505	BCR	C34-C9-C10	-3.22	118.41	122.92
15	A	1107	CLA	CMA-C3A-C4A	3.22	120.43	111.77
15	3	606	CLA	C2C-C1C-NC	3.22	112.99	109.97
16	2	611	CHL	CMA-C3A-C4A	3.22	120.42	111.77
15	A	1107	CLA	C2C-C1C-NC	3.22	112.98	109.97
15	B	1204	CLA	C2C-C1C-NC	3.22	112.98	109.97
15	B	1214	CLA	C2C-C1C-NC	3.21	112.98	109.97
15	4	615	CLA	CMA-C3A-C4A	3.21	120.41	111.77
16	4	610	CHL	CMA-C3A-C4A	3.21	120.40	111.77
15	A	1013	CLA	C2C-C1C-NC	3.21	112.98	109.97
16	2	610	CHL	CMA-C3A-C4A	3.21	120.39	111.77
15	A	1101	CLA	C2C-C1C-NC	3.20	112.97	109.97
15	4	615	CLA	C2C-C1C-NC	3.20	112.97	109.97
16	2	609	CHL	CMA-C3A-C4A	3.20	120.38	111.77
13	3	502	XAT	C15-C14-C13	-3.20	122.75	127.31
12	3	501	LUT	C31-C30-C29	-3.20	122.75	127.31
16	2	610	CHL	C3C-C4C-NC	-3.19	106.99	110.57
16	2	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1106	CLA	C2C-C1C-NC	3.19	112.96	109.97
15	B	1240	CLA	C2C-C1C-NC	3.19	112.96	109.97
15	4	609	CLA	CMA-C3A-C4A	3.19	120.34	111.77
14	A	4003	BCR	C34-C9-C10	-3.19	118.46	122.92
15	B	1210	CLA	C2C-C1C-NC	3.18	112.95	109.97
14	3	504	BCR	C33-C5-C4	3.18	119.72	113.62
14	B	4005	BCR	C15-C14-C13	-3.17	122.78	127.31
16	3	604	CHL	CHD-C4C-C3C	3.17	129.50	124.84
14	A	4004	BCR	C33-C5-C4	3.17	119.71	113.62
15	2	605	CLA	CMA-C3A-C4A	3.17	120.29	111.77
14	B	4001	BCR	C1-C6-C5	-3.17	118.15	122.61
16	4	613	CHL	C3C-C4C-NC	-3.17	107.02	110.57
15	2	607	CLA	C2C-C1C-NC	3.16	112.94	109.97
15	3	601	CLA	CMA-C3A-C4A	3.16	120.27	111.77
14	4	503	BCR	C27-C26-C25	-3.16	118.14	122.73
15	A	1123	CLA	C2C-C1C-NC	3.16	112.93	109.97
14	B	4004	BCR	C27-C26-C25	-3.16	118.14	122.73
15	B	1209	CLA	C2C-C1C-NC	3.16	112.93	109.97
15	A	1137	CLA	CMA-C3A-C4A	3.16	120.26	111.77
14	J	4003	BCR	C27-C26-C25	-3.16	118.15	122.73
15	1	608	CLA	CMA-C3A-C4A	3.16	120.26	111.77
15	B	1230	CLA	C2C-C1C-NC	3.16	112.93	109.97
16	1	609	CHL	C3C-C4C-NC	-3.16	107.03	110.57
14	B	4004	BCR	C33-C5-C4	3.15	119.67	113.62
16	4	611	CHL	C2C-C3C-C4C	3.15	108.74	106.49
14	A	4002	BCR	C33-C5-C4	3.15	119.67	113.62
21	B	5002	DGD	O1G-C1A-C2A	3.15	119.64	111.38
15	B	1217	CLA	CMA-C3A-C4A	3.15	120.23	111.77
15	A	1124	CLA	C2C-C1C-NC	3.15	112.92	109.97
16	2	611	CHL	C3C-C4C-NC	-3.15	107.04	110.57
15	3	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
15	2	602	CLA	C2C-C1C-NC	3.14	112.92	109.97
14	4	503	BCR	C38-C26-C27	3.14	119.65	113.62
15	B	1224	CLA	C2C-C1C-NC	3.14	112.92	109.97
15	B	1231	CLA	C2C-C1C-NC	3.14	112.91	109.97
15	A	1012	CLA	C2C-C1C-NC	3.14	112.91	109.97
14	3	503	BCR	C27-C26-C25	-3.14	118.18	122.73
15	3	603	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
15	A	1140	CLA	CMA-C3A-C4A	3.14	120.20	111.77
15	B	1021	CLA	C2C-C1C-NC	3.13	112.91	109.97
15	A	1103	CLA	C1-C2-C3	-3.13	120.62	126.04
15	A	1130	CLA	C2C-C1C-NC	3.13	112.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	503	BCR	C36-C18-C17	-3.13	118.54	122.92
16	3	604	CHL	CMA-C3A-C4A	3.13	120.19	111.77
14	J	4002	BCR	C27-C26-C25	-3.13	118.19	122.73
15	B	1219	CLA	C2C-C1C-NC	3.13	112.90	109.97
13	3	502	XAT	O4-C5-C18	-3.13	111.31	115.06
15	B	1226	CLA	CMA-C3A-C4A	3.12	120.17	111.77
15	F	1302	CLA	C2C-C1C-NC	3.12	112.90	109.97
15	B	1239	CLA	C1-C2-C3	-3.12	120.64	126.04
12	2	501	LUT	C22-C23-C24	-3.12	108.19	111.74
15	A	1114	CLA	C2C-C1C-NC	3.12	112.89	109.97
15	A	1121	CLA	C2C-C1C-NC	3.11	112.89	109.97
15	A	1116	CLA	C2C-C1C-NC	3.11	112.89	109.97
14	F	4002	BCR	C33-C5-C4	3.11	119.59	113.62
15	4	605	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
15	B	1211	CLA	CMA-C3A-C4A	3.11	120.12	111.77
15	2	603	CLA	CMA-C3A-C4A	3.11	120.12	111.77
15	1	611	CLA	C2C-C1C-NC	3.10	112.88	109.97
14	B	4001	BCR	C4-C5-C6	-3.10	118.23	122.73
15	2	605	CLA	C2C-C1C-NC	3.10	112.88	109.97
15	B	1222	CLA	C2C-C1C-NC	3.10	112.88	109.97
15	A	1135	CLA	CMA-C3A-C4A	3.10	120.11	111.77
15	A	1141	CLA	C2C-C1C-NC	3.10	112.87	109.97
15	A	1139	CLA	CMA-C3A-C4A	3.09	120.09	111.77
15	A	1132	CLA	C2C-C1C-NC	3.09	112.87	109.97
14	A	4007	BCR	C27-C26-C25	-3.09	118.24	122.73
14	A	4007	BCR	C36-C18-C17	-3.09	118.59	122.92
14	1	503	BCR	C38-C26-C27	3.09	119.55	113.62
15	B	1210	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	B	1237	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	B	1205	CLA	CMA-C3A-C4A	3.09	120.07	111.77
15	3	607	CLA	C2C-C1C-NC	3.09	112.86	109.97
16	2	613	CHL	CMA-C3A-C4A	3.08	120.06	111.77
14	B	4005	BCR	C38-C26-C25	-3.08	121.06	124.53
15	B	1237	CLA	C2C-C1C-NC	3.08	112.86	109.97
15	B	1212	CLA	C2C-C1C-NC	3.08	112.86	109.97
15	2	608	CLA	CMA-C3A-C4A	3.08	120.05	111.77
14	A	4003	BCR	C33-C5-C4	3.08	119.53	113.62
14	1	503	BCR	C34-C9-C10	-3.07	118.62	122.92
15	A	1119	CLA	C2C-C1C-NC	3.07	112.85	109.97
15	B	1220	CLA	CMA-C3A-C4A	3.07	120.03	111.77
15	A	1129	CLA	C2C-C1C-NC	3.07	112.85	109.97
14	B	4003	BCR	C34-C9-C10	-3.07	118.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	503	BCR	C28-C27-C26	-3.07	108.60	114.08
15	B	1215	CLA	C2C-C1C-NC	3.07	112.84	109.97
15	1	607	CLA	C2C-C1C-NC	3.07	112.84	109.97
15	B	1235	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	B	1238	CLA	CMA-C3A-C4A	3.06	120.00	111.77
15	3	611	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	B	1230	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	A	1134	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	B	1238	CLA	C2C-C1C-NC	3.06	112.84	109.97
15	4	608	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	B	1206	CLA	CMA-C3A-C4A	3.06	119.98	111.77
15	A	1137	CLA	C2C-C1C-NC	3.05	112.83	109.97
15	A	1101	CLA	CMA-C3A-C4A	3.05	119.98	111.77
15	B	1232	CLA	C2C-C1C-NC	3.05	112.83	109.97
15	B	1235	CLA	CMA-C3A-C4A	3.05	119.98	111.77
14	1	503	BCR	C27-C26-C25	-3.05	118.30	122.73
15	2	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
14	F	4002	BCR	C27-C26-C25	-3.05	118.30	122.73
16	1	610	CHL	C3C-C4C-NC	-3.05	107.15	110.57
15	B	1204	CLA	CMA-C3A-C4A	3.05	119.97	111.77
15	1	605	CLA	CMA-C3A-C4A	3.05	119.96	111.77
14	4	503	BCR	C33-C5-C4	3.05	119.47	113.62
14	J	4001	BCR	C33-C5-C4	3.05	119.47	113.62
15	B	1218	CLA	CMA-C3A-C4A	3.04	119.96	111.77
15	2	615	CLA	C2C-C1C-NC	3.04	112.82	109.97
12	1	501	LUT	C39-C29-C30	-3.04	118.66	122.92
15	B	1218	CLA	C2C-C1C-NC	3.04	112.82	109.97
15	B	1206	CLA	C2C-C1C-NC	3.04	112.82	109.97
14	B	4002	BCR	C27-C26-C25	-3.04	118.32	122.73
15	A	1125	CLA	CMA-C3A-C4A	3.04	119.95	111.77
15	3	603	CLA	CMA-C3A-C4A	3.04	119.94	111.77
15	A	1139	CLA	C6-C5-C3	-3.04	109.65	114.62
15	3	607	CLA	CMA-C3A-C4A	3.04	119.94	111.77
16	4	611	CHL	C3C-C4C-NC	-3.04	107.16	110.57
15	A	1112	CLA	CMA-C3A-C4A	3.04	119.94	111.77
15	A	1117	CLA	C2C-C1C-NC	3.04	112.82	109.97
15	B	1232	CLA	CMA-C3A-C4A	3.04	119.93	111.77
15	1	608	CLA	C2C-C1C-NC	3.03	112.81	109.97
14	A	4002	BCR	C36-C18-C17	-3.03	118.67	122.92
15	1	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
15	A	1120	CLA	CMA-C3A-C4A	3.03	119.92	111.77
14	B	4001	BCR	C23-C24-C25	-3.03	118.69	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	608	CLA	CMA-C3A-C4A	3.03	119.91	111.77
14	B	4005	BCR	C23-C24-C25	-3.03	118.70	127.20
15	A	1130	CLA	CMA-C3A-C4A	3.03	119.91	111.77
15	A	1106	CLA	C1-C2-C3	-3.03	120.81	126.04
15	B	1239	CLA	CMA-C3A-C4A	3.03	119.91	111.77
15	A	1111	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
15	A	1123	CLA	CMA-C3A-C4A	3.02	119.89	111.77
15	B	1228	CLA	C2C-C1C-NC	3.02	112.80	109.97
15	B	1234	CLA	C2C-C1C-NC	3.02	112.80	109.97
25	B	2002	PQN	C14-C13-C15	3.02	120.34	115.27
14	J	4003	BCR	C30-C25-C26	-3.02	118.37	122.61
15	B	1227	CLA	CMA-C3A-C4A	3.02	119.88	111.77
15	B	1222	CLA	CMA-C3A-C4A	3.01	119.88	111.77
15	A	1126	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
15	A	1116	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	A	1131	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	J	1302	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	B	1240	CLA	CMA-C3A-C4A	3.01	119.87	111.77
15	A	1136	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	B	1221	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1115	CLA	CMA-C3A-C4A	3.01	119.86	111.77
14	1	505	BCR	C30-C25-C26	-3.01	118.38	122.61
15	B	1219	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1141	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1121	CLA	CMA-C3A-C4A	3.01	119.85	111.77
15	B	1220	CLA	C2C-C1C-NC	3.00	112.79	109.97
15	A	1125	CLA	C2C-C1C-NC	3.00	112.79	109.97
14	1	505	BCR	C35-C13-C14	-3.00	118.72	122.92
14	A	4006	BCR	C23-C24-C25	-3.00	118.77	127.20
15	4	603	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	B	1203	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	A	1113	CLA	CMA-C3A-C4A	3.00	119.83	111.77
15	A	1109	CLA	C2C-C1C-NC	3.00	112.78	109.97
15	B	1203	CLA	C2C-C1C-NC	2.99	112.78	109.97
15	A	1105	CLA	C2C-C1C-NC	2.99	112.78	109.97
15	A	1120	CLA	C2C-C1C-NC	2.99	112.78	109.97
15	A	1129	CLA	CMA-C3A-C4A	2.99	119.81	111.77
15	3	610	CLA	C2C-C1C-NC	2.99	112.77	109.97
15	A	1104	CLA	CMA-C3A-C4A	2.99	119.81	111.77
15	B	1227	CLA	C2C-C1C-NC	2.99	112.77	109.97
15	3	612	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	3	605	CLA	C2C-C1C-NC	2.99	112.77	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	B	1223	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	A	1118	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	A	1139	CLA	C2C-C1C-NC	2.98	112.77	109.97
15	A	1132	CLA	CMA-C3A-C4A	2.98	119.79	111.77
15	B	1201	CLA	C2C-C1C-NC	2.98	112.77	109.97
15	A	1122	CLA	CMA-C3A-C4A	2.98	119.78	111.77
15	B	1217	CLA	C2C-C1C-NC	2.98	112.76	109.97
14	4	505	BCR	C27-C26-C25	-2.98	118.41	122.73
12	2	501	LUT	C31-C30-C29	-2.98	123.06	127.31
15	3	605	CLA	CMA-C3A-C4A	2.97	119.77	111.77
25	A	2001	PQN	C14-C13-C15	2.97	120.27	115.27
14	B	4003	BCR	C27-C26-C25	-2.97	118.42	122.73
15	B	1209	CLA	CMA-C3A-C4A	2.97	119.76	111.77
15	1	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
15	A	1138	CLA	C2C-C1C-NC	2.97	112.75	109.97
15	A	1117	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	2	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	A	1122	CLA	C2C-C1C-NC	2.97	112.75	109.97
14	3	504	BCR	C27-C26-C25	-2.97	118.42	122.73
15	3	610	CLA	CMA-C3A-C4A	2.97	119.75	111.77
15	A	1124	CLA	CMA-C3A-C4A	2.96	119.74	111.77
15	B	1228	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	A	1108	CLA	C2C-C1C-NC	2.96	112.75	109.97
15	A	1111	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	1	615	CLA	CMA-C3A-C4A	2.96	119.73	111.77
15	A	1101	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
14	A	4007	BCR	C34-C9-C10	-2.96	118.78	122.92
15	J	1302	CLA	C2C-C1C-NC	2.96	112.74	109.97
15	B	1201	CLA	CMA-C3A-C4A	2.96	119.72	111.77
15	B	1022	CLA	C2C-C1C-NC	2.96	112.74	109.97
15	B	1229	CLA	CMA-C3A-C4A	2.96	119.72	111.77
14	A	4006	BCR	C27-C26-C25	-2.96	118.44	122.73
15	B	1225	CLA	CMA-C3A-C4A	2.96	119.72	111.77
15	B	1224	CLA	CMA-C3A-C4A	2.95	119.71	111.77
15	1	615	CLA	C1-C2-C3	-2.95	120.94	126.04
15	A	1127	CLA	CMA-C3A-C4A	2.95	119.71	111.77
12	4	501	LUT	C31-C30-C29	-2.95	123.10	127.31
12	2	501	LUT	C18-C5-C4	2.95	119.82	114.36
15	B	1205	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	A	1011	CL0	CAA-C2A-C3A	-2.94	104.72	112.78
14	A	4005	BCR	C23-C24-C25	-2.94	118.94	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	607	CLA	CMA-C3A-C4A	2.94	119.68	111.77
15	B	1240	CLA	C1-C2-C3	-2.94	120.96	126.04
15	A	1113	CLA	C2C-C1C-NC	2.94	112.72	109.97
15	A	1110	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	B	1215	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	B	1202	CLA	CMA-C3A-C4A	2.93	119.66	111.77
15	B	1213	CLA	C2C-C1C-NC	2.93	112.72	109.97
15	1	611	CLA	CMA-C3A-C4A	2.93	119.65	111.77
12	4	501	LUT	C21-C26-C27	2.93	116.41	112.70
15	A	1134	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	A	1105	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	A	1126	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	4	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	2	615	CLA	CMA-C3A-C4A	2.92	119.63	111.77
15	1	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	3	613	CLA	CMA-C3A-C4A	2.92	119.62	111.77
14	B	4004	BCR	C30-C25-C26	-2.92	118.50	122.61
15	2	612	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	B	1236	CLA	C2C-C1C-NC	2.92	112.71	109.97
15	A	1108	CLA	CMA-C3A-C4A	2.91	119.60	111.77
15	B	1212	CLA	CMA-C3A-C4A	2.91	119.60	111.77
15	1	612	CLA	CMA-C3A-C4A	2.91	119.59	111.77
15	1	602	CLA	C2C-C1C-NC	2.91	112.70	109.97
15	2	607	CLA	CMA-C3A-C4A	2.91	119.59	111.77
15	1	607	CLA	CMA-C3A-C4A	2.91	119.59	111.77
14	A	4003	BCR	C19-C18-C17	2.91	123.40	118.94
15	B	1208	CLA	C2C-C1C-NC	2.91	112.70	109.97
15	3	601	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1102	CLA	C2C-C1C-NC	2.90	112.69	109.97
14	B	4006	BCR	C33-C5-C4	2.90	119.19	113.62
16	2	611	CHL	C2C-C3C-C4C	2.90	108.56	106.49
15	4	601	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	4	602	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	F	1301	CLA	CMA-C3A-C4A	2.90	119.57	111.77
14	1	505	BCR	C27-C26-C25	-2.90	118.52	122.73
15	4	607	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1128	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	4	612	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	2	604	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	A	1133	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A	1133	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	A	1119	CLA	CMA-C3A-C4A	2.90	119.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	611	CHL	C4D-C3D-CAD	-2.90	106.86	108.47
15	B	1234	CLA	CMA-C3A-C4A	2.89	119.55	111.77
15	4	604	CLA	C2C-C1C-NC	2.89	112.68	109.97
14	A	4005	BCR	C30-C25-C26	-2.89	118.54	122.61
15	A	1118	CLA	C2C-C1C-NC	2.89	112.68	109.97
15	A	1131	CLA	C2C-C1C-NC	2.89	112.68	109.97
15	B	1229	CLA	C2C-C1C-NC	2.89	112.68	109.97
16	1	609	CHL	C2C-C3C-C4C	2.89	108.55	106.49
15	3	608	CLA	C2C-C1C-NC	2.88	112.67	109.97
15	A	1114	CLA	CMA-C3A-C4A	2.88	119.52	111.77
15	3	615	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
15	A	1109	CLA	CMA-C3A-C4A	2.88	119.52	111.77
15	1	601	CLA	CMA-C3A-C4A	2.88	119.52	111.77
15	B	1236	CLA	CMA-C3A-C4A	2.88	119.51	111.77
15	A	1013	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
16	4	611	CHL	CMA-C3A-C4A	2.88	119.51	111.77
14	J	4003	BCR	C33-C5-C4	2.88	119.14	113.62
16	3	604	CHL	C1B-CHB-C4A	-2.88	124.42	130.12
15	1	603	CLA	CMA-C3A-C4A	2.87	119.50	111.77
15	1	601	CLA	C2C-C1C-NC	2.87	112.67	109.97
15	2	605	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
15	1	613	CLA	CMA-C3A-C4A	2.87	119.49	111.77
14	A	4007	BCR	C33-C5-C4	2.87	119.13	113.62
15	1	602	CLA	CMA-C3A-C4A	2.87	119.48	111.77
15	B	1022	CLA	CMA-C3A-C4A	2.87	119.47	111.77
14	4	505	BCR	C38-C26-C27	2.86	119.12	113.62
16	2	609	CHL	C2C-C3C-C4C	2.86	108.53	106.49
15	2	603	CLA	C2C-C1C-NC	2.86	112.65	109.97
15	1	605	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
15	3	612	CLA	C2C-C1C-NC	2.86	112.65	109.97
14	4	505	BCR	C35-C13-C14	-2.86	118.92	122.92
14	A	4007	BCR	C23-C24-C25	-2.85	119.19	127.20
14	J	4003	BCR	C38-C26-C27	2.85	119.10	113.62
15	A	1103	CLA	CMA-C3A-C4A	2.85	119.44	111.77
15	A	1105	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	B	1226	CLA	C2C-C1C-NC	2.85	112.64	109.97
15	B	1219	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
15	A	1102	CLA	CMA-C3A-C4A	2.85	119.43	111.77
15	B	1208	CLA	CMA-C3A-C4A	2.85	119.42	111.77
15	A	1130	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
14	F	4002	BCR	C34-C9-C10	-2.84	118.94	122.92
15	B	1213	CLA	CMA-C3A-C4A	2.84	119.41	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	601	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
15	3	615	CLA	CMA-C3A-C4A	2.84	119.41	111.77
14	B	4001	BCR	C34-C9-C10	-2.84	118.94	122.92
14	B	4002	BCR	C38-C26-C27	2.84	119.07	113.62
15	F	1301	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
15	B	1210	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
15	1	603	CLA	C2C-C1C-NC	2.83	112.62	109.97
14	A	4005	BCR	C38-C26-C27	2.83	119.05	113.62
15	3	611	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
15	2	601	CLA	C2C-C1C-NC	2.83	112.62	109.97
14	J	4001	BCR	C38-C26-C27	2.83	119.05	113.62
15	B	1023	CLA	CMA-C3A-C4A	2.83	119.37	111.77
15	B	1223	CLA	C1C-C2C-C3C	-2.83	103.99	106.96
15	B	1216	CLA	C2C-C1C-NC	2.82	112.62	109.97
14	3	503	BCR	C38-C26-C27	2.82	119.04	113.62
15	4	605	CLA	CMA-C3A-C4A	2.82	119.36	111.77
13	4	502	XAT	C6-C7-C8	-2.82	120.03	125.99
14	A	4002	BCR	C38-C26-C27	2.82	119.04	113.62
15	4	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
15	A	1108	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
15	4	603	CLA	C2C-C1C-NC	2.82	112.61	109.97
15	B	1202	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
13	3	502	XAT	C26-C27-C28	-2.82	120.04	125.99
15	A	1109	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
15	A	1104	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
16	2	613	CHL	C4D-C3D-CAD	-2.81	106.90	108.47
15	B	1214	CLA	CMA-C3A-C4A	2.81	119.33	111.77
15	B	1229	CLA	O2A-CGA-CBA	2.81	120.73	111.91
15	B	1239	CLA	C2C-C1C-NC	2.81	112.61	109.97
15	B	1021	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
16	3	604	CHL	C2C-C3C-C4C	2.81	108.49	106.49
13	4	502	XAT	C26-C27-C28	-2.81	120.06	125.99
12	3	501	LUT	C22-C23-C24	-2.80	108.55	111.74
15	B	1235	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
14	1	505	BCR	C15-C14-C13	-2.80	123.31	127.31
15	B	1225	CLA	C2C-C1C-NC	2.80	112.60	109.97
15	4	604	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
14	B	4002	BCR	C23-C24-C25	-2.80	119.34	127.20
15	4	605	CLA	C2C-C1C-NC	2.80	112.59	109.97
15	A	1128	CLA	CMA-C3A-C4A	2.79	119.28	111.77
16	4	610	CHL	C2C-C3C-C4C	2.79	108.48	106.49
15	4	609	CLA	C1C-C2C-C3C	-2.79	104.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	505	BCR	C4-C5-C6	-2.79	118.68	122.73
15	A	1108	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
15	A	1103	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
15	1	608	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
15	B	1216	CLA	CMA-C3A-C4A	2.78	119.25	111.77
15	A	1110	CLA	C2C-C1C-NC	2.78	112.58	109.97
15	1	606	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
15	4	602	CLA	C2C-C1C-NC	2.78	112.58	109.97
13	2	502	XAT	O24-C25-C38	-2.78	111.73	115.06
14	B	4001	BCR	C38-C26-C27	2.78	118.95	113.62
14	B	4004	BCR	C38-C26-C27	2.77	118.94	113.62
14	3	503	BCR	C30-C25-C26	-2.77	118.71	122.61
15	2	601	CLA	CMA-C3A-C4A	2.77	119.23	111.77
13	4	502	XAT	C38-C25-C26	-2.77	117.62	122.26
15	B	1023	CLA	O2A-CGA-CBA	2.77	120.60	111.91
14	A	4007	BCR	C38-C26-C27	2.77	118.94	113.62
15	A	1106	CLA	CMA-C3A-C4A	2.77	119.22	111.77
15	B	1207	CLA	C3D-C4D-ND	2.77	112.55	110.14
13	3	502	XAT	C35-C15-C14	-2.77	117.80	123.47
15	4	608	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
15	A	1135	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
14	A	4006	BCR	C33-C5-C4	2.77	118.93	113.62
15	2	606	CLA	CMA-C3A-C4A	2.77	119.21	111.77
15	A	1107	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
14	A	4005	BCR	C35-C13-C14	-2.76	119.06	122.92
15	2	612	CLA	CMA-C3A-C4A	2.76	119.19	111.77
15	B	1207	CLA	C3A-C4A-CHB	2.76	127.29	123.91
14	3	504	BCR	C38-C26-C27	2.75	118.91	113.62
13	1	502	XAT	C38-C25-C26	-2.75	117.64	122.26
15	B	1230	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	1	615	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
15	1	606	CLA	CAA-C2A-C1A	-2.75	102.96	111.97
14	J	4001	BCR	C23-C24-C25	-2.75	119.48	127.20
15	A	1140	CLA	C2C-C1C-NC	2.75	112.55	109.97
15	3	613	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
14	A	4007	BCR	C8-C9-C10	2.74	123.15	118.94
15	B	1214	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
12	4	501	LUT	C8-C7-C6	-2.74	119.50	127.20
15	1	613	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
14	B	4004	BCR	C23-C24-C25	-2.73	119.52	127.20
15	3	605	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
14	J	4002	BCR	C38-C26-C27	2.73	118.86	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1119	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
15	A	1141	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
16	1	610	CHL	C4D-C3D-CAD	-2.73	106.95	108.47
14	1	505	BCR	C38-C26-C27	2.73	118.86	113.62
14	A	4002	BCR	C37-C22-C21	-2.73	119.10	122.92
15	B	1206	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
16	1	609	CHL	C1B-CHB-C4A	-2.72	124.72	130.12
14	2	503	BCR	C27-C26-C25	-2.72	118.78	122.73
14	1	503	BCR	C37-C22-C23	2.72	122.37	118.08
14	A	4002	BCR	C30-C25-C26	-2.72	118.78	122.61
24	A	1011	CL0	CMC-C2C-C1C	2.72	129.19	125.04
14	4	503	BCR	C30-C25-C26	-2.72	118.78	122.61
14	J	4002	BCR	C30-C25-C26	-2.72	118.78	122.61
15	B	1203	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
15	4	604	CLA	CMA-C3A-C4A	2.72	119.08	111.77
16	4	613	CHL	C4D-C3D-CAD	-2.72	106.96	108.47
15	A	1115	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
16	1	609	CHL	C1-O2A-CGA	2.71	123.56	116.44
15	A	1124	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
21	2	811	DGD	O1G-C1A-C2A	2.71	120.42	111.91
15	2	605	CLA	OBD-CAD-C3D	-2.71	123.48	127.98
21	4	811	DGD	C2G-O2G-C1B	-2.71	111.12	117.79
18	1	802	LMG	C8-O7-C10	-2.71	111.12	117.79
16	1	610	CHL	CHC-C1C-NC	2.71	128.31	124.20
13	2	502	XAT	C6-C7-C8	-2.71	120.27	125.99
21	B	5002	DGD	C2G-O2G-C1B	-2.70	111.13	117.79
15	B	1211	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
15	B	1223	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	F	1302	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
15	B	1231	CLA	CMA-C3A-C4A	2.70	119.03	111.77
14	B	4003	BCR	C38-C26-C27	2.70	118.80	113.62
14	J	4003	BCR	C23-C24-C25	-2.70	119.63	127.20
15	B	1218	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
15	B	1222	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
14	4	505	BCR	C1-C6-C5	-2.70	118.81	122.61
15	A	1104	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
14	A	4007	BCR	C19-C18-C17	2.70	123.08	118.94
21	4	811	DGD	O1G-C1A-C2A	2.70	120.37	111.91
15	A	1136	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
14	B	4001	BCR	C30-C25-C26	-2.69	118.82	122.61
14	1	503	BCR	C36-C18-C17	-2.69	119.15	122.92
15	A	1013	CLA	OBD-CAD-C3D	-2.69	123.51	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1216	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	B	1240	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	A	1140	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	A	1112	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
14	J	4001	BCR	C30-C25-C26	-2.69	118.83	122.61
15	A	1128	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	1	503	BCR	C35-C13-C12	2.69	122.31	118.08
15	A	1123	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	B	1224	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
15	A	1106	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
14	4	503	BCR	C34-C9-C10	-2.69	119.16	122.92
15	2	602	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
15	A	1116	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
15	B	1222	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	A	1011	CL0	CAC-C3C-C4C	2.68	128.29	124.81
15	2	607	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	B	1226	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	B	1205	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	3	606	CLA	CMA-C3A-C4A	2.68	118.98	111.77
14	A	4006	BCR	C35-C13-C12	2.68	122.30	118.08
15	B	1215	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	3	601	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
15	F	1302	CLA	CMA-C3A-C4A	2.68	118.97	111.77
15	A	1103	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
17	B	5001	LHG	C5-O7-C7	-2.68	112.91	117.90
13	1	502	XAT	C19-C9-C10	-2.67	119.18	122.92
15	2	606	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
13	3	502	XAT	C40-C33-C34	-2.67	119.18	122.92
16	4	611	CHL	C1B-CHB-C4A	-2.67	124.83	130.12
15	A	1132	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
16	3	604	CHL	C4D-C3D-CAD	-2.67	106.98	108.47
15	3	612	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	B	1022	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
15	3	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
14	2	503	BCR	C38-C26-C27	2.67	118.74	113.62
15	1	602	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	A	1121	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
15	A	1137	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
15	A	1132	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
24	A	1011	CL0	C5-C3-C4	2.66	120.48	114.60
14	3	504	BCR	C8-C7-C6	-2.66	119.74	127.20
15	A	1117	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	603	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
15	A	1012	CLA	CMA-C3A-C4A	2.65	118.90	111.77
15	3	601	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
14	B	4003	BCR	C30-C25-C26	-2.65	118.88	122.61
14	A	4003	BCR	C8-C9-C10	2.65	123.01	118.94
15	B	1220	CLA	C1-C2-C3	-2.65	121.47	126.04
13	3	502	XAT	C38-C25-C26	-2.64	117.83	122.26
15	4	607	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
15	A	1126	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
15	3	607	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
15	B	1023	CLA	C1-C2-C3	-2.64	121.48	126.04
16	2	611	CHL	C4A-NA-C1A	2.64	107.89	106.71
14	F	4002	BCR	C38-C26-C27	2.64	118.68	113.62
14	B	4001	BCR	C1-C6-C7	2.64	123.23	115.78
15	2	612	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
14	A	4006	BCR	C30-C25-C26	-2.63	118.91	122.61
15	B	1220	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
15	B	1023	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
25	A	2001	PQN	C2M-C2-C3	-2.63	120.11	124.40
16	4	613	CHL	C1-O2A-CGA	2.63	123.34	116.44
16	2	610	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
15	4	607	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
15	A	1012	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
15	4	606	CLA	C2C-C1C-NC	2.62	112.43	109.97
15	B	1234	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
15	B	1235	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	1	802	LMG	O8-C28-C29	2.62	120.13	111.91
16	3	604	CHL	CHC-C1C-NC	2.62	128.18	124.20
15	A	1134	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
15	1	604	CLA	CMA-C3A-C4A	2.62	118.81	111.77
17	1	801	LHG	C5-O7-C7	-2.62	111.35	117.79
14	B	4006	BCR	C36-C18-C17	-2.62	119.26	122.92
15	2	604	CLA	O2A-CGA-CBA	2.61	120.11	111.91
12	4	501	LUT	C31-C32-C33	-2.61	119.08	126.42
15	B	1237	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
15	A	1138	CLA	O2A-CGA-CBA	2.61	120.10	111.91
15	2	608	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
15	2	615	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
15	1	615	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	B	4004	BCR	C34-C9-C10	-2.61	119.27	122.92
14	J	4003	BCR	C34-C9-C10	-2.61	119.27	122.92
15	B	1221	CLA	C1C-C2C-C3C	-2.60	104.22	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1012	CLA	O2A-CGA-CBA	2.60	120.08	111.91
15	1	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
15	A	1115	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	4	505	BCR	C37-C22-C21	-2.60	119.28	122.92
16	2	613	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
15	A	1127	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
15	A	1137	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
12	3	501	LUT	C18-C5-C4	2.60	119.17	114.36
15	A	1012	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	B	4002	BCR	C34-C9-C10	-2.59	119.29	122.92
16	1	610	CHL	CHD-C4C-C3C	2.59	128.65	124.84
15	B	1215	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
14	A	4006	BCR	C38-C26-C27	2.59	118.59	113.62
15	B	1204	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
15	A	1139	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
14	2	503	BCR	C36-C18-C17	-2.59	119.30	122.92
15	2	604	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
15	2	602	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
16	2	610	CHL	C2C-C3C-C4C	2.57	108.32	106.49
16	2	610	CHL	C4D-C3D-CAD	-2.57	107.03	108.47
15	B	1228	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	B	4001	BCR	C35-C13-C14	-2.57	119.32	122.92
15	A	1104	CLA	O2A-CGA-CBA	2.57	119.98	111.91
13	1	502	XAT	C18-C5-C6	-2.57	117.95	122.26
15	A	1101	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
15	B	1238	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
14	A	4004	BCR	C37-C22-C21	-2.57	119.32	122.92
15	1	601	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
15	4	606	CLA	CMA-C3A-C4A	2.57	118.67	111.77
15	A	1114	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
14	3	504	BCR	C30-C25-C26	-2.57	119.00	122.61
15	4	615	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
14	J	4001	BCR	C35-C13-C12	2.56	122.11	118.08
25	B	2002	PQN	C2M-C2-C3	-2.56	120.23	124.40
15	1	605	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	A	1117	CLA	O2A-CGA-CBA	2.55	119.92	111.91
15	A	1139	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
15	3	608	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
12	1	501	LUT	C7-C8-C9	-2.55	122.38	126.23
15	A	1129	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
15	2	608	CLA	O2A-CGA-CBA	2.54	119.89	111.91
15	4	602	CLA	O2D-CGD-O1D	-2.54	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	610	CHL	C1B-CHB-C4A	-2.54	125.08	130.12
14	J	4003	BCR	C35-C13-C12	2.54	122.08	118.08
14	4	505	BCR	C30-C25-C26	-2.54	119.03	122.61
15	4	604	CLA	O2A-CGA-CBA	2.54	119.89	111.91
14	3	503	BCR	C8-C7-C6	-2.54	120.07	127.20
15	1	611	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
15	A	1125	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
15	B	1201	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
15	4	609	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
15	4	605	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
15	A	1127	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	B	1236	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	A	1102	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
15	2	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	A	4002	BCR	C34-C9-C8	2.52	122.05	118.08
15	B	1021	CLA	CMA-C3A-C4A	2.52	118.55	111.77
15	2	601	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
15	A	1136	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
14	A	4005	BCR	C4-C5-C6	-2.52	119.08	122.73
15	A	1133	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
15	A	1111	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	4	606	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
15	A	1113	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
14	1	505	BCR	C37-C22-C21	-2.51	119.40	122.92
15	B	1240	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
15	1	606	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
15	1	607	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
15	B	1209	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
15	B	1229	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
14	A	4002	BCR	C19-C18-C17	2.50	122.78	118.94
15	B	1239	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
15	B	1235	CLA	O2A-CGA-CBA	2.50	119.74	111.91
15	B	1232	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
15	B	1211	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
15	A	1120	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
15	A	1114	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	1	503	BCR	C4-C5-C6	-2.49	119.11	122.73
23	B	5031	GSH	CG1-CD1-N2	2.49	120.15	115.83
15	A	1123	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
15	B	1023	CLA	C2C-C1C-NC	2.49	112.30	109.97
14	F	4002	BCR	C36-C18-C17	-2.49	119.44	122.92
15	4	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1122	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
15	A	1109	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	B	1229	CLA	C1-C2-C3	-2.48	121.76	126.04
15	B	1225	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
16	1	610	CHL	C2C-C3C-C4C	2.48	108.25	106.49
15	A	1111	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
15	B	1239	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
21	2	811	DGD	C2G-O2G-C1B	-2.48	111.70	117.79
15	B	1205	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
15	3	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	J	1302	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1118	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1110	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
14	1	505	BCR	C34-C9-C10	-2.47	119.46	122.92
15	B	1220	CLA	O2A-CGA-CBA	2.47	119.66	111.91
14	F	4002	BCR	C30-C25-C26	-2.47	119.13	122.61
15	3	603	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
15	1	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	F	1302	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
15	A	1134	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
13	1	502	XAT	C26-C27-C28	-2.46	120.79	125.99
14	A	4003	BCR	C35-C13-C12	2.46	121.95	118.08
18	2	802	LMG	C8-O7-C10	-2.46	111.73	117.79
15	B	1209	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
12	1	501	LUT	C8-C7-C6	-2.46	120.30	127.20
14	1	503	BCR	C3-C4-C5	-2.46	109.69	114.08
15	A	1121	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
15	B	1022	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
14	B	4003	BCR	C8-C9-C10	2.45	122.71	118.94
15	1	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
16	4	611	CHL	C4A-NA-C1A	2.45	107.81	106.71
14	3	503	BCR	C4-C5-C6	-2.45	119.17	122.73
14	A	4006	BCR	C34-C9-C10	-2.45	119.49	122.92
14	3	504	BCR	C37-C22-C21	-2.45	119.49	122.92
15	F	1301	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
16	4	610	CHL	CHD-C4C-C3C	2.44	128.43	124.84
15	B	1212	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
12	1	501	LUT	C28-C29-C30	2.44	122.69	118.94
15	A	1131	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	B	1230	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	1	612	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	B	1208	CLA	C1C-C2C-C3C	-2.44	104.39	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	4003	BCR	C36-C18-C17	-2.44	119.51	122.92
15	B	1217	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
15	B	1210	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
14	B	4005	BCR	C34-C9-C10	-2.44	119.51	122.92
15	B	1230	CLA	O2A-CGA-CBA	2.43	119.55	111.91
14	4	503	BCR	C36-C18-C17	-2.43	119.51	122.92
15	3	607	CLA	O2A-CGA-CBA	2.43	119.55	111.91
15	4	601	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	A	1108	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
15	B	1227	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
14	A	4007	BCR	C30-C25-C26	-2.43	119.19	122.61
23	4	831	GSH	CG1-CD1-N2	2.43	120.04	115.83
15	4	601	CLA	O2A-CGA-CBA	2.43	119.52	111.91
14	B	4003	BCR	C15-C14-C13	-2.43	123.85	127.31
15	3	615	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
15	1	604	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
14	A	4007	BCR	C35-C13-C14	-2.42	119.53	122.92
15	B	1213	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
15	A	1131	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
14	J	4002	BCR	C35-C13-C14	-2.42	119.53	122.92
15	4	601	CLA	C2C-C1C-NC	2.42	112.24	109.97
15	A	1105	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
15	1	604	CLA	O2A-CGA-CBA	2.42	119.49	111.91
14	A	4006	BCR	C36-C18-C19	2.42	121.88	118.08
15	4	612	CLA	O2A-CGA-CBA	2.41	119.48	111.91
16	4	610	CHL	C4D-C3D-CAD	-2.41	107.12	108.47
16	2	610	CHL	C4A-NA-C1A	2.41	107.79	106.71
15	A	1124	CLA	O2A-CGA-CBA	2.41	119.47	111.91
24	A	1011	CL0	CMB-C2B-C3B	2.41	129.18	124.68
15	A	1127	CLA	O2A-CGA-CBA	2.40	119.45	111.91
15	A	1013	CLA	CBA-CAA-C2A	-2.40	106.77	113.86
14	A	4003	BCR	C38-C26-C25	-2.40	121.83	124.53
15	B	1240	CLA	O2A-CGA-CBA	2.40	119.43	111.91
15	3	607	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	B	1227	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
15	A	1141	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
14	4	503	BCR	C30-C25-C24	2.40	122.55	115.78
16	4	611	CHL	C1-O2A-CGA	2.39	122.72	116.44
15	A	1135	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	1	606	CLA	C2C-C1C-NC	2.39	112.21	109.97
15	B	1221	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	B	1227	CLA	CAA-CBA-CGA	-2.39	108.46	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1226	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
15	A	1122	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
15	B	1231	CLA	O2A-CGA-CBA	2.39	119.40	111.91
15	A	1113	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
14	3	503	BCR	C15-C14-C13	-2.38	123.91	127.31
16	2	613	CHL	CHD-C4C-C3C	2.38	128.34	124.84
15	A	1110	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
15	B	1232	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	B	1237	CLA	O2A-CGA-CBA	2.38	119.37	111.91
14	B	4006	BCR	C38-C26-C27	2.37	118.18	113.62
12	2	501	LUT	C8-C7-C6	-2.37	120.53	127.20
15	A	1101	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
15	4	605	CLA	O2A-CGA-CBA	2.37	119.34	111.91
13	4	502	XAT	C18-C5-C6	-2.37	118.29	122.26
15	1	604	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
15	A	1139	CLA	C1-O2A-CGA	2.37	122.65	116.44
15	A	1120	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
13	1	502	XAT	C40-C33-C34	-2.36	119.61	122.92
15	B	1210	CLA	O2A-CGA-CBA	2.36	119.33	111.91
15	A	1116	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
15	B	1231	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
15	A	1126	CLA	O2A-CGA-CBA	2.36	119.32	111.91
14	2	503	BCR	C30-C25-C26	-2.36	119.29	122.61
15	3	612	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
15	3	603	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	B	1213	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
15	2	607	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
16	4	610	CHL	CHB-C4A-NA	2.36	127.77	124.51
13	4	502	XAT	O4-C5-C18	-2.36	112.23	115.06
13	3	502	XAT	C19-C9-C10	-2.35	119.62	122.92
15	1	611	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
14	A	4004	BCR	C38-C26-C27	2.35	118.13	113.62
15	B	1022	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
15	3	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	A	1106	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
15	B	1216	CLA	O2A-CGA-CBA	2.35	119.29	111.91
22	2	821	LMT	C3'-C4'-C5'	-2.35	105.54	110.93
15	B	1218	CLA	O2A-CGA-CBA	2.35	119.28	111.91
15	B	1204	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	B	1224	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
15	B	1234	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
14	F	4002	BCR	C35-C13-C14	-2.35	119.64	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1239	CLA	O2A-CGA-CBA	2.34	119.26	111.91
12	2	501	LUT	C15-C35-C34	-2.34	118.67	123.47
15	2	603	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
14	B	4006	BCR	C34-C9-C10	-2.34	119.64	122.92
15	A	1118	CLA	O2A-CGA-CBA	2.34	119.26	111.91
15	3	608	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
14	3	503	BCR	C19-C18-C17	2.34	122.53	118.94
15	B	1215	CLA	O2A-CGA-CBA	2.34	119.25	111.91
13	1	502	XAT	C20-C13-C14	-2.33	119.65	122.92
15	3	611	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
15	3	606	CLA	CAA-CBA-CGA	-2.33	108.57	113.59
15	4	605	CLA	OBD-CAD-C3D	-2.33	124.11	127.98
15	4	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	B	1238	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	B	1225	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
15	A	1102	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
15	A	1124	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
15	2	605	CLA	CHA-C1A-NA	-2.33	121.06	126.40
15	B	1023	CLA	CHA-C1A-NA	-2.33	121.06	126.40
14	B	4003	BCR	C36-C18-C17	-2.33	119.66	122.92
15	B	1220	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
12	3	501	LUT	C19-C9-C10	-2.33	119.67	122.92
15	2	615	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
12	1	501	LUT	C18-C5-C4	2.32	118.66	114.36
15	B	1201	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
15	A	1130	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
16	1	609	CHL	CHC-C1C-NC	2.32	127.72	124.20
15	4	612	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
15	A	1120	CLA	O2A-CGA-CBA	2.32	119.18	111.91
14	A	4002	BCR	C23-C24-C25	-2.32	120.69	127.20
15	B	1212	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
16	1	610	CHL	CMD-C2D-C3D	2.31	129.01	124.68
15	B	1229	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
15	A	1138	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
15	4	603	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
15	B	1226	CLA	O2A-CGA-CBA	2.31	119.16	111.91
15	B	1218	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	B	1214	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	2	615	CLA	O2A-CGA-CBA	2.31	119.16	111.91
15	A	1107	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	A	1119	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
12	1	501	LUT	C22-C23-C24	-2.31	109.12	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	609	CHL	C4D-C3D-CAD	-2.31	107.18	108.47
15	A	1013	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
15	A	1139	CLA	O2A-CGA-CBA	2.30	119.14	111.91
15	2	608	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
15	4	608	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	A	1119	CLA	O2A-CGA-CBA	2.30	119.13	111.91
15	A	1112	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	3	610	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	A	1123	CLA	O2A-CGA-CBA	2.30	119.12	111.91
16	2	609	CHL	C1B-CHB-C4A	-2.30	125.57	130.12
14	4	505	BCR	C8-C9-C10	2.30	122.46	118.94
16	4	613	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
16	2	610	CHL	CHD-C4C-C3C	2.29	128.21	124.84
16	3	604	CHL	CMD-C2D-C3D	2.29	128.97	124.68
14	4	505	BCR	C15-C14-C13	-2.29	124.04	127.31
15	4	607	CLA	O2A-CGA-CBA	2.29	119.10	111.91
15	A	1013	CLA	O2A-CGA-CBA	2.29	119.10	111.91
14	B	4001	BCR	C3-C4-C5	-2.29	109.99	114.08
15	B	1203	CLA	O2A-CGA-CBA	2.29	119.09	111.91
15	B	1228	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
15	A	1118	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	1	811	SQD	O3-C3-C2	-2.29	105.06	110.35
12	2	501	LUT	C19-C9-C10	-2.28	119.72	122.92
13	4	502	XAT	O24-C25-C24	2.28	115.10	113.38
14	J	4002	BCR	C23-C24-C25	-2.28	120.79	127.20
12	2	501	LUT	C11-C12-C13	-2.28	120.00	126.42
15	A	1117	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
14	B	4006	BCR	C15-C14-C13	-2.28	124.06	127.31
15	A	1128	CLA	O2A-CGA-CBA	2.28	119.05	111.91
16	2	609	CHL	C4D-C3D-CAD	-2.28	107.20	108.47
15	2	602	CLA	O2A-CGA-CBA	2.28	119.05	111.91
16	1	609	CHL	C4A-NA-C1A	2.28	107.73	106.71
15	2	606	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
15	2	603	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
15	3	606	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
16	2	611	CHL	C1B-CHB-C4A	-2.27	125.62	130.12
13	2	502	XAT	C38-C25-C26	-2.27	118.46	122.26
16	2	610	CHL	C1-O2A-CGA	2.27	122.39	116.44
15	B	1206	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
15	2	612	CLA	O2A-CGA-CBA	2.26	119.01	111.91
15	A	1132	CLA	O2A-CGA-CBA	2.26	119.01	111.91
15	A	1111	CLA	CHA-C1A-NA	-2.26	121.21	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1237	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	J	4001	BCR	C36-C18-C17	-2.26	119.75	122.92
14	4	503	BCR	C37-C22-C21	-2.26	119.76	122.92
14	1	505	BCR	C12-C13-C14	2.26	122.41	118.94
14	1	503	BCR	C23-C22-C21	-2.26	115.48	118.94
15	B	1236	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
14	B	4006	BCR	C28-C27-C26	-2.26	110.05	114.08
16	1	609	CHL	CMD-C2D-C3D	2.25	128.90	124.68
15	A	1013	CLA	CMA-C3A-C4A	2.25	117.83	111.77
15	B	1206	CLA	O2A-CGA-CBA	2.25	118.98	111.91
14	B	4002	BCR	C36-C18-C17	-2.25	119.77	122.92
12	4	501	LUT	C10-C11-C12	-2.25	116.20	123.22
16	2	611	CHL	C4D-C3D-CAD	-2.25	107.22	108.47
15	4	606	CLA	O2A-CGA-CBA	2.25	118.96	111.91
15	4	603	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	3	601	CLA	O2A-CGA-CBA	2.25	118.96	111.91
15	A	1129	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	B	1021	CLA	O2A-CGA-CBA	2.24	118.95	111.91
15	A	1105	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
15	B	1231	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	3	605	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
16	2	610	CHL	CMD-C2D-C3D	2.24	128.87	124.68
14	A	4004	BCR	C8-C7-C6	-2.24	120.91	127.20
15	1	605	CLA	O2A-CGA-CBA	2.24	118.93	111.91
14	F	4002	BCR	C23-C24-C25	-2.24	120.92	127.20
15	A	1122	CLA	O2A-CGA-CBA	2.24	118.92	111.91
14	B	4001	BCR	C36-C18-C17	-2.23	119.79	122.92
15	B	1236	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
13	4	502	XAT	C40-C33-C34	-2.23	119.79	122.92
15	2	604	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
16	1	610	CHL	C1-O2A-CGA	2.23	123.47	116.11
15	B	1221	CLA	O2A-CGA-CBA	2.23	118.91	111.91
15	J	1302	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
15	A	1128	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	1	603	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	B	1214	CLA	O2A-CGA-CBA	2.23	118.91	111.91
15	A	1121	CLA	O2A-CGA-CBA	2.23	118.90	111.91
15	2	612	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
15	B	1208	CLA	O2A-CGA-CBA	2.22	118.89	111.91
15	B	1228	CLA	O2A-CGA-CBA	2.22	118.89	111.91
15	3	606	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
15	1	607	CLA	O2D-CGD-O1D	-2.22	119.49	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4002	BCR	C30-C25-C26	-2.22	119.49	122.61
15	B	1202	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
15	1	611	CLA	O2A-CGA-CBA	2.22	118.87	111.91
15	A	1140	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
15	3	610	CLA	O2A-CGA-CBA	2.22	118.87	111.91
15	A	1134	CLA	O2A-CGA-CBA	2.22	118.86	111.91
13	2	502	XAT	O4-C5-C18	-2.22	112.40	115.06
15	2	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	A	1133	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
15	B	1207	CLA	C2C-C3C-C4C	-2.21	104.56	107.21
15	A	1103	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	B	1216	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
14	3	504	BCR	C23-C24-C25	-2.21	120.99	127.20
16	2	609	CHL	CMB-C2B-C1B	-2.21	125.06	128.46
14	2	503	BCR	C34-C9-C10	-2.21	119.83	122.92
15	B	1022	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	A	1135	CLA	O2A-CGA-CBA	2.21	118.83	111.91
14	F	4002	BCR	C37-C22-C21	-2.20	119.83	122.92
15	1	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
15	4	601	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
16	2	613	CHL	CMB-C2B-C1B	-2.20	125.08	128.46
14	A	4005	BCR	C8-C7-C6	-2.20	121.02	127.20
15	A	1124	CLA	C1-O2A-CGA	2.20	122.21	116.44
15	B	1204	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
15	4	607	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	A	1012	CLA	CHA-C1A-NA	-2.20	121.37	126.40
15	2	601	CLA	O2A-CGA-CBA	2.20	118.80	111.91
15	B	1202	CLA	O2A-CGA-CBA	2.19	118.80	111.91
16	1	610	CHL	CMB-C2B-C1B	-2.19	125.09	128.46
14	B	4005	BCR	C38-C26-C27	2.19	117.83	113.62
12	2	501	LUT	C20-C13-C14	-2.19	119.85	122.92
15	B	1236	CLA	O2A-CGA-CBA	2.19	118.78	111.91
12	4	501	LUT	C38-C25-C24	-2.19	118.88	123.56
15	F	1302	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	A	1141	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	3	606	CLA	CHA-C1A-NA	-2.19	121.39	126.40
15	3	603	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
19	1	811	SQD	O8-S-C6	-2.19	102.25	105.74
14	B	4003	BCR	C23-C24-C25	-2.19	121.06	127.20
15	A	1131	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	F	1301	CLA	O2A-CGA-CBA	2.19	118.77	111.91
15	1	613	CLA	CHA-C1A-NA	-2.18	121.40	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	C27-C28-C29	2.18	128.92	125.53
15	4	609	CLA	CHA-C1A-NA	-2.18	121.40	126.40
15	A	1112	CLA	O2A-CGA-CBA	2.18	118.75	111.91
15	A	1130	CLA	O2A-CGA-CBA	2.18	118.75	111.91
15	B	1204	CLA	O2A-CGA-CBA	2.18	118.74	111.91
16	4	611	CHL	CMD-C2D-C3D	2.18	128.75	124.68
15	B	1215	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
15	A	1116	CLA	O2A-CGA-CBA	2.18	118.73	111.91
15	B	1213	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B	1217	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
15	3	608	CLA	O2A-CGA-CBA	2.17	118.72	111.91
17	A	5002	LHG	O7-C7-O9	-2.17	118.45	123.70
15	1	612	CLA	O2A-CGA-CBA	2.17	118.72	111.91
15	A	1101	CLA	CHA-C1A-NA	-2.17	121.43	126.40
15	1	606	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
15	B	1201	CLA	O2A-CGA-CBA	2.17	118.72	111.91
15	B	1208	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
14	A	4003	BCR	C38-C26-C27	2.17	117.78	113.62
16	2	611	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
13	3	502	XAT	O24-C25-C24	2.16	115.01	113.38
15	2	607	CLA	O2A-CGA-CBA	2.16	118.69	111.91
15	A	1136	CLA	O2A-CGA-CBA	2.16	118.69	111.91
14	1	503	BCR	C12-C13-C14	-2.16	115.63	118.94
13	1	502	XAT	C39-C29-C30	-2.16	119.90	122.92
15	2	601	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	A	1137	CLA	O2A-CGA-CBA	2.16	118.67	111.91
14	A	4003	BCR	C37-C22-C21	-2.16	119.90	122.92
14	4	503	BCR	C3-C4-C5	-2.16	110.23	114.08
15	B	1223	CLA	CHA-C1A-NA	-2.15	121.47	126.40
16	3	604	CHL	CHB-C4A-NA	2.15	127.49	124.51
14	B	4002	BCR	C37-C22-C21	-2.15	119.91	122.92
15	B	1221	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
15	A	1133	CLA	O2A-CGA-CBA	2.15	118.66	111.91
15	B	1219	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
15	B	1023	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
15	A	1129	CLA	O2A-CGA-CBA	2.15	118.66	111.91
14	B	4005	BCR	C28-C27-C26	-2.15	110.24	114.08
16	2	611	CHL	CMD-C2D-C3D	2.15	128.70	124.68
14	A	4006	BCR	C12-C13-C14	-2.15	115.64	118.94
15	3	612	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	A	1111	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	A	1110	CLA	CHA-C1A-NA	-2.15	121.48	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	503	BCR	C8-C7-C6	-2.15	121.18	127.20
16	2	611	CHL	C1-O2A-CGA	2.15	122.96	116.73
15	A	1103	CLA	O2A-CGA-CBA	2.15	118.64	111.91
15	B	1229	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
15	B	1213	CLA	O2A-CGA-CBA	2.14	118.63	111.91
15	B	1205	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
15	B	1228	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	A	1115	CLA	O2A-CGA-CBA	2.14	118.62	111.91
16	2	611	CHL	CHC-C1C-NC	2.14	127.45	124.20
15	3	601	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
24	A	1011	CL0	O2D-CGD-O1D	-2.14	119.66	123.84
16	4	613	CHL	CHB-C4A-NA	2.14	127.47	124.51
14	A	4004	BCR	C38-C26-C25	-2.14	122.13	124.53
18	1	802	LMG	O7-C10-O9	-2.14	118.54	123.70
14	J	4003	BCR	C7-C6-C5	-2.14	116.29	121.46
15	A	1106	CLA	O2A-CGA-CBA	2.14	118.61	111.91
15	4	607	CLA	OBD-CAD-C3D	-2.13	124.44	127.98
13	3	502	XAT	C18-C5-C6	-2.13	118.69	122.26
15	1	605	CLA	OBD-CAD-C3D	-2.13	124.44	127.98
14	F	4002	BCR	C8-C9-C10	2.13	122.21	118.94
15	B	1225	CLA	O2A-CGA-CBA	2.13	118.60	111.91
16	2	609	CHL	CMD-C2D-C3D	2.13	128.66	124.68
15	B	1219	CLA	O2A-CGA-CBA	2.13	118.59	111.91
15	B	1223	CLA	O2A-CGA-CBA	2.13	118.59	111.91
14	1	503	BCR	C38-C26-C25	-2.13	122.14	124.53
16	2	613	CHL	CMD-C2D-C3D	2.13	128.66	124.68
15	4	601	CLA	C1-O2A-CGA	2.13	122.02	116.44
16	2	609	CHL	CHC-C1C-NC	2.13	127.43	124.20
16	2	611	CHL	CHB-C4A-NA	2.12	127.45	124.51
15	4	602	CLA	O2A-CGA-CBA	2.12	118.57	111.91
14	B	4004	BCR	C36-C18-C17	-2.12	119.95	122.92
15	4	601	CLA	CHA-C1A-NA	-2.12	121.54	126.40
14	A	4004	BCR	C28-C27-C26	-2.12	110.29	114.08
14	A	4006	BCR	C8-C7-C6	-2.12	121.25	127.20
15	B	1023	CLA	CMB-C2B-C3B	2.12	128.64	124.68
15	2	608	CLA	C1-O2A-CGA	2.12	122.00	116.44
16	1	609	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
15	B	1021	CLA	C1-O2A-CGA	2.12	122.00	116.44
15	B	1212	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
14	A	4002	BCR	C35-C13-C12	2.12	121.41	118.08
15	B	1224	CLA	O2A-CGA-CBA	2.12	118.55	111.91
15	A	1107	CLA	O2A-CGA-CBA	2.12	118.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1137	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
14	J	4002	BCR	C36-C18-C17	-2.11	119.96	122.92
15	A	1109	CLA	CHA-C1A-NA	-2.11	121.56	126.40
16	2	609	CHL	CHD-C4C-C3C	2.11	127.94	124.84
15	A	1101	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
12	1	501	LUT	C38-C25-C24	-2.11	119.04	123.56
14	J	4003	BCR	C37-C22-C21	-2.11	119.97	122.92
15	A	1108	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
15	B	1234	CLA	O2A-CGA-CBA	2.11	118.53	111.91
16	3	604	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
15	B	1214	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
15	2	605	CLA	O2A-CGA-CBA	2.10	118.51	111.91
15	A	1112	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	4	615	CLA	CHA-C1A-NA	-2.10	121.58	126.40
16	2	610	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
16	4	611	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
16	4	613	CHL	CHD-C4C-C3C	2.10	127.93	124.84
15	A	1124	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	1	601	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
15	B	1236	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	1	601	CLA	CHA-C1A-NA	-2.10	121.60	126.40
15	4	612	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
15	2	601	CLA	OBD-CAD-C3D	-2.10	124.50	127.98
15	A	1137	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B	1226	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
15	3	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B	1022	CLA	C1-O2A-CGA	2.09	121.93	116.44
16	4	610	CHL	CMD-C2D-C3D	2.09	128.59	124.68
12	4	501	LUT	C7-C8-C9	-2.09	123.08	126.23
16	2	613	CHL	C4A-NA-C1A	2.09	107.64	106.71
15	A	1139	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	4	612	CLA	CHA-C1A-NA	-2.09	121.62	126.40
14	J	4002	BCR	C3-C4-C5	-2.09	110.35	114.08
15	A	1102	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
15	B	1238	CLA	CHA-C1A-NA	-2.08	121.62	126.40
15	2	606	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
15	B	1240	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	A	1125	CLA	O2A-CGA-CBA	2.08	118.44	111.91
15	B	1209	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	B	1216	CLA	CHA-C1A-NA	-2.08	121.63	126.40
14	F	4002	BCR	C31-C1-C6	-2.08	106.92	110.30
15	F	1302	CLA	CHA-C1A-NA	-2.08	121.63	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	615	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
14	B	4006	BCR	C19-C18-C17	2.08	122.13	118.94
14	2	503	BCR	C4-C5-C6	-2.08	119.72	122.73
15	B	1217	CLA	CHA-C1A-NA	-2.07	121.65	126.40
14	4	503	BCR	C38-C26-C25	-2.07	122.20	124.53
15	A	1105	CLA	O2A-CGA-CBA	2.07	118.42	111.91
15	A	1134	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
15	2	605	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
14	A	4004	BCR	C27-C26-C25	-2.07	119.72	122.73
15	B	1022	CLA	O2A-CGA-CBA	2.07	118.41	111.91
15	A	1111	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
15	1	602	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	1	604	CLA	C1-O2A-CGA	2.07	121.88	116.44
13	2	502	XAT	C19-C9-C10	-2.07	120.02	122.92
15	B	1214	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	1	606	CLA	CMB-C2B-C3B	2.07	128.54	124.68
13	4	502	XAT	C39-C29-C30	-2.07	120.03	122.92
14	3	504	BCR	C35-C13-C14	-2.07	120.03	122.92
15	A	1110	CLA	C1-O2A-CGA	2.06	121.86	116.44
15	B	1220	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	B	1220	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
14	3	503	BCR	C34-C9-C10	-2.06	120.03	122.92
15	B	1213	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
15	1	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	2	601	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
15	B	1223	CLA	OBD-CAD-C3D	-2.06	124.57	127.98
15	4	601	CLA	CMB-C2B-C3B	2.06	128.52	124.68
15	A	1108	CLA	CHA-C1A-NA	-2.05	121.69	126.40
15	A	1132	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
14	2	503	BCR	C1-C6-C7	2.05	121.59	115.78
15	B	1219	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	B	1205	CLA	O2A-CGA-CBA	2.05	118.35	111.91
16	4	610	CHL	C1-O2A-CGA	2.05	122.87	116.11
13	1	502	XAT	O4-C5-C4	-2.05	111.84	113.38
12	4	501	LUT	C18-C5-C4	2.05	118.16	114.36
14	J	4002	BCR	C37-C22-C21	-2.05	120.05	122.92
16	2	610	CHL	CHC-C1C-NC	2.05	127.31	124.20
15	1	605	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
15	1	605	CLA	CAA-CBA-CGA	-2.05	107.27	113.25
15	A	1123	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	4	603	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	B	1224	CLA	CHA-C1A-NA	-2.05	121.71	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1109	CLA	O2A-CGA-CBA	2.05	118.33	111.91
15	A	1115	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
15	A	1125	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
15	B	1212	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A	1013	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A	1127	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	4	603	CLA	O2A-CGA-CBA	2.04	118.32	111.91
15	3	607	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	B	1229	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A	1120	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	3	603	CLA	CAC-C3C-C2C	-2.04	124.04	127.53
15	2	605	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
14	B	4003	BCR	C37-C22-C21	-2.04	120.07	122.92
15	B	1234	CLA	CHA-C1A-NA	-2.04	121.73	126.40
15	B	1021	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
15	B	1225	CLA	CHA-C1A-NA	-2.04	121.73	126.40
16	1	609	CHL	CHD-C4C-C3C	2.04	127.83	124.84
15	B	1234	CLA	C1-O2A-CGA	2.03	121.78	116.44
14	3	504	BCR	C34-C9-C10	-2.03	120.07	122.92
14	J	4002	BCR	C33-C5-C6	-2.03	122.25	124.53
15	4	606	CLA	CHA-C1A-NA	-2.03	121.74	126.40
16	2	609	CHL	C1-O2A-CGA	2.03	121.78	116.44
15	A	1119	CLA	CHA-C1A-NA	-2.03	121.75	126.40
14	2	503	BCR	C23-C24-C25	-2.03	121.50	127.20
15	B	1021	CLA	CHA-C1A-NA	-2.03	121.75	126.40
16	4	613	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
12	3	501	LUT	C40-C33-C34	-2.03	120.08	122.92
15	3	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40
15	2	602	CLA	CHA-C1A-NA	-2.03	121.76	126.40
15	B	1212	CLA	CAA-CBA-CGA	-2.02	109.24	113.59
15	3	615	CLA	CHA-C1A-NA	-2.02	121.76	126.40
15	A	1104	CLA	C1-O2A-CGA	2.02	121.75	116.44
15	B	1231	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
15	B	1222	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
15	B	1237	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
14	B	4002	BCR	C35-C13-C14	-2.02	120.09	122.92
15	A	1127	CLA	C1-O2A-CGA	2.02	121.75	116.44
15	4	604	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	4	602	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	4	615	CLA	O2A-CGA-CBA	2.02	118.24	111.91
15	B	1235	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
15	A	1113	CLA	CHA-C1A-NA	-2.02	121.78	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1129	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	1	601	CLA	O2A-CGA-CBA	2.02	118.23	111.91
15	B	1232	CLA	O2A-CGA-CBA	2.02	118.23	111.91
16	1	610	CHL	C4A-NA-C1A	2.02	107.61	106.71
15	B	1208	CLA	CHA-C1A-NA	-2.01	121.78	126.40
12	1	501	LUT	C19-C9-C8	2.01	121.25	118.08
15	B	1221	CLA	CHA-C1A-NA	-2.01	121.78	126.40
15	2	608	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
15	4	609	CLA	O2A-CGA-CBA	2.01	118.22	111.91
13	2	502	XAT	C18-C5-C6	-2.01	118.89	122.26
15	3	603	CLA	C1D-CHD-C4C	2.01	125.21	122.56
16	4	613	CHL	CMD-C2D-C3D	2.01	128.44	124.68
15	B	1218	CLA	CHA-C1A-NA	-2.01	121.80	126.40
12	4	501	LUT	C19-C9-C8	2.01	121.24	118.08
16	2	613	CHL	CHB-C4A-NA	2.01	127.29	124.51
15	B	1206	CLA	CHA-C1A-NA	-2.01	121.80	126.40
16	4	610	CHL	CMB-C2B-C1B	-2.01	125.38	128.46
15	A	1111	CLA	CMC-C2C-C1C	2.01	128.09	125.04
16	2	611	CHL	CHD-C4C-C3C	2.01	127.79	124.84
16	2	613	CHL	CHC-C1C-NC	2.01	127.25	124.20
15	1	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	B	1227	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
14	A	4005	BCR	C37-C22-C21	-2.00	120.12	122.92
15	A	1138	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
17	1	801	LHG	O7-C7-O9	-2.00	118.87	123.70

All (438) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	4	604	CLA	NC
15	4	604	CLA	ND
15	4	604	CLA	NA
15	A	1124	CLA	NC
15	A	1124	CLA	ND
15	A	1124	CLA	NA
15	A	1133	CLA	NC
15	A	1133	CLA	ND
15	A	1133	CLA	NA
15	2	608	CLA	NC
15	2	608	CLA	ND
15	2	608	CLA	NA
13	3	502	XAT	C6

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Mol	Chain	Res	Type	Atom
15	2	601	CLA	NC
15	2	601	CLA	ND
15	2	601	CLA	NA
15	B	1218	CLA	NC
15	B	1218	CLA	ND
15	B	1218	CLA	NA
15	A	1119	CLA	NC
15	A	1119	CLA	ND
15	A	1119	CLA	NA
15	A	1127	CLA	NC
15	A	1127	CLA	ND
15	A	1127	CLA	NA
15	A	1134	CLA	NC
15	A	1134	CLA	ND
15	A	1134	CLA	NA
15	A	1130	CLA	NC
15	A	1130	CLA	ND
15	A	1130	CLA	NA
15	B	1205	CLA	NC
15	B	1205	CLA	ND
15	B	1205	CLA	NA
15	A	1117	CLA	NC
15	A	1117	CLA	ND
15	A	1117	CLA	NA
15	A	1013	CLA	NC
15	A	1013	CLA	ND
15	A	1013	CLA	NA
15	F	1301	CLA	NC
15	F	1301	CLA	ND
15	F	1301	CLA	NA
15	B	1213	CLA	NC
15	B	1213	CLA	ND
15	B	1213	CLA	NA
15	3	612	CLA	NC
15	3	612	CLA	ND
15	3	612	CLA	NA
15	1	601	CLA	NC
15	1	601	CLA	ND
15	1	601	CLA	NA
16	3	604	CHL	NC
16	3	604	CHL	ND
16	3	604	CHL	NA

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Mol	Chain	Res	Type	Atom
15	B	1227	CLA	NC
15	B	1227	CLA	ND
15	B	1227	CLA	NA
15	A	1108	CLA	NC
15	A	1108	CLA	ND
15	A	1108	CLA	NA
15	B	1214	CLA	NC
15	B	1214	CLA	ND
15	B	1214	CLA	NA
15	4	601	CLA	NC
15	4	601	CLA	ND
15	4	601	CLA	NA
15	B	1229	CLA	NC
15	B	1229	CLA	ND
15	B	1229	CLA	NA
15	3	607	CLA	NC
15	3	607	CLA	ND
15	3	607	CLA	NA
15	B	1209	CLA	NC
15	B	1209	CLA	ND
15	B	1209	CLA	NA
16	4	610	CHL	NC
16	4	610	CHL	ND
16	4	610	CHL	NA
16	4	610	CHL	C3A
15	4	607	CLA	NC
15	4	607	CLA	ND
15	4	607	CLA	NA
15	B	1204	CLA	NC
15	B	1204	CLA	ND
15	B	1204	CLA	NA
15	A	1136	CLA	NC
15	A	1136	CLA	ND
15	A	1136	CLA	NA
15	B	1211	CLA	NC
15	B	1211	CLA	ND
15	B	1211	CLA	NA
15	A	1109	CLA	NC
15	A	1109	CLA	ND
15	A	1109	CLA	NA
15	A	1113	CLA	NC
15	A	1113	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1113	CLA	NA
15	4	608	CLA	NC
15	4	608	CLA	ND
15	4	608	CLA	NA
15	A	1122	CLA	NC
15	A	1122	CLA	ND
15	A	1122	CLA	NA
15	2	602	CLA	NC
15	2	602	CLA	ND
15	2	602	CLA	NA
16	4	613	CHL	NC
16	4	613	CHL	ND
16	4	613	CHL	NA
16	4	613	CHL	C3A
15	2	607	CLA	NC
15	2	607	CLA	ND
15	2	607	CLA	NA
15	B	1230	CLA	NC
15	B	1230	CLA	ND
15	B	1230	CLA	NA
15	3	613	CLA	NC
15	3	613	CLA	ND
15	3	613	CLA	NA
15	1	604	CLA	NC
15	1	604	CLA	ND
15	1	604	CLA	NA
15	2	604	CLA	NC
15	2	604	CLA	ND
15	2	604	CLA	NA
15	A	1138	CLA	NC
15	A	1138	CLA	ND
15	A	1138	CLA	NA
15	A	1128	CLA	NC
15	A	1128	CLA	ND
15	A	1128	CLA	NA
15	J	1302	CLA	NC
15	J	1302	CLA	ND
15	J	1302	CLA	NA
15	B	1231	CLA	NC
15	B	1231	CLA	ND
15	B	1231	CLA	NA
13	4	502	XAT	C6

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Mol	Chain	Res	Type	Atom
15	A	1118	CLA	NC
15	A	1118	CLA	ND
15	A	1118	CLA	NA
15	4	615	CLA	NC
15	4	615	CLA	ND
15	4	615	CLA	NA
15	A	1129	CLA	NC
15	A	1129	CLA	ND
15	A	1129	CLA	NA
15	B	1215	CLA	NC
15	B	1215	CLA	ND
15	B	1215	CLA	NA
15	4	605	CLA	NC
15	4	605	CLA	ND
15	4	605	CLA	NA
15	B	1224	CLA	NC
15	B	1224	CLA	ND
15	B	1224	CLA	NA
15	A	1104	CLA	NC
15	A	1104	CLA	ND
15	A	1104	CLA	NA
15	B	1202	CLA	NC
15	B	1202	CLA	ND
15	B	1202	CLA	NA
15	2	612	CLA	NC
15	2	612	CLA	ND
15	2	612	CLA	NA
15	A	1115	CLA	NC
15	A	1115	CLA	ND
15	A	1115	CLA	NA
15	3	605	CLA	NC
15	3	605	CLA	ND
15	3	605	CLA	NA
15	A	1114	CLA	NC
15	A	1114	CLA	ND
15	A	1114	CLA	NA
15	B	1022	CLA	NC
15	B	1022	CLA	ND
15	B	1022	CLA	NA
15	3	615	CLA	NC
15	3	615	CLA	ND
15	3	615	CLA	NA

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Mol	Chain	Res	Type	Atom
15	B	1203	CLA	NC
15	B	1203	CLA	ND
15	B	1203	CLA	NA
15	1	613	CLA	NC
15	1	613	CLA	ND
15	1	613	CLA	NA
15	B	1207	CLA	NC
15	B	1207	CLA	ND
15	B	1207	CLA	NA
15	B	1220	CLA	NC
15	B	1220	CLA	ND
15	B	1220	CLA	NA
15	3	610	CLA	NC
15	3	610	CLA	ND
15	3	610	CLA	NA
15	A	1123	CLA	NC
15	A	1123	CLA	ND
15	A	1123	CLA	NA
15	B	1236	CLA	NC
15	B	1236	CLA	ND
15	B	1236	CLA	NA
15	A	1111	CLA	NC
15	A	1111	CLA	ND
15	A	1111	CLA	NA
15	4	606	CLA	NC
15	4	606	CLA	ND
15	4	606	CLA	NA
15	B	1206	CLA	NC
15	B	1206	CLA	ND
15	B	1206	CLA	NA
15	1	602	CLA	NC
15	1	602	CLA	ND
15	1	602	CLA	NA
15	B	1226	CLA	NC
15	B	1226	CLA	ND
15	B	1226	CLA	NA
15	B	1239	CLA	NC
15	B	1239	CLA	ND
15	B	1239	CLA	NA
15	B	1216	CLA	NC
15	B	1216	CLA	ND
15	B	1216	CLA	NA

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Mol	Chain	Res	Type	Atom
15	A	1012	CLA	NC
15	A	1012	CLA	ND
15	A	1012	CLA	NA
15	A	1110	CLA	NC
15	A	1110	CLA	ND
15	A	1110	CLA	NA
15	A	1132	CLA	NC
15	A	1132	CLA	ND
15	A	1132	CLA	NA
16	2	609	CHL	NC
16	2	609	CHL	ND
16	2	609	CHL	NA
15	B	1240	CLA	NC
15	B	1240	CLA	ND
15	B	1240	CLA	NA
15	B	1217	CLA	NC
15	B	1217	CLA	ND
15	B	1217	CLA	NA
15	4	602	CLA	NC
15	4	602	CLA	ND
15	4	602	CLA	NA
15	1	606	CLA	NC
15	1	606	CLA	ND
15	1	606	CLA	NA
15	B	1021	CLA	NC
15	B	1021	CLA	ND
15	B	1021	CLA	NA
15	4	612	CLA	NC
15	4	612	CLA	ND
15	4	612	CLA	NA
15	1	611	CLA	NC
15	1	611	CLA	ND
15	1	611	CLA	NA
15	B	1235	CLA	NC
15	B	1235	CLA	ND
15	B	1235	CLA	NA
15	3	601	CLA	NC
15	3	601	CLA	ND
15	3	601	CLA	NA
13	2	502	XAT	C26
15	B	1223	CLA	NC
15	B	1223	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1223	CLA	NA
15	A	1107	CLA	NC
15	A	1107	CLA	ND
15	A	1107	CLA	NA
15	A	1120	CLA	NC
15	A	1120	CLA	ND
15	A	1120	CLA	NA
15	A	1141	CLA	NC
15	A	1141	CLA	ND
15	A	1141	CLA	NA
15	B	1228	CLA	NC
15	B	1228	CLA	ND
15	B	1228	CLA	NA
16	1	610	CHL	NC
16	1	610	CHL	ND
16	1	610	CHL	NA
15	2	605	CLA	NC
15	2	605	CLA	ND
15	2	605	CLA	NA
15	B	1222	CLA	NC
15	B	1222	CLA	ND
15	B	1222	CLA	NA
15	1	612	CLA	C13
15	1	612	CLA	NC
15	1	612	CLA	ND
15	1	612	CLA	NA
15	2	615	CLA	NC
15	2	615	CLA	ND
15	2	615	CLA	NA
15	A	1140	CLA	NC
15	A	1140	CLA	ND
15	A	1140	CLA	NA
15	4	603	CLA	NC
15	4	603	CLA	ND
15	4	603	CLA	NA
15	B	1023	CLA	NC
15	B	1023	CLA	ND
15	B	1023	CLA	NA
15	B	1210	CLA	NC
15	B	1210	CLA	ND
15	B	1210	CLA	NA
15	1	615	CLA	NC

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Mol	Chain	Res	Type	Atom
15	1	615	CLA	ND
15	1	615	CLA	NA
15	4	609	CLA	NC
15	4	609	CLA	ND
15	4	609	CLA	NA
15	A	1116	CLA	NC
15	A	1116	CLA	ND
15	A	1116	CLA	NA
15	B	1234	CLA	NC
15	B	1234	CLA	ND
15	B	1234	CLA	NA
15	B	1221	CLA	NC
15	B	1221	CLA	ND
15	B	1221	CLA	NA
16	2	611	CHL	NC
16	2	611	CHL	ND
16	2	611	CHL	NA
16	2	611	CHL	C3A
15	B	1219	CLA	NC
15	B	1219	CLA	ND
15	B	1219	CLA	NA
15	A	1126	CLA	NC
15	A	1126	CLA	ND
15	A	1126	CLA	NA
15	2	603	CLA	NC
15	2	603	CLA	ND
15	2	603	CLA	NA
15	A	1112	CLA	NC
15	A	1112	CLA	ND
15	A	1112	CLA	NA
15	A	1139	CLA	NC
15	A	1139	CLA	ND
15	A	1139	CLA	NA
15	B	1201	CLA	NC
15	B	1201	CLA	ND
15	B	1201	CLA	NA
15	1	603	CLA	NC
15	1	603	CLA	ND
15	1	603	CLA	NA
15	B	1225	CLA	NC
15	B	1225	CLA	ND
15	B	1225	CLA	NA

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Mol	Chain	Res	Type	Atom
15	F	1302	CLA	NC
15	F	1302	CLA	ND
15	F	1302	CLA	NA
15	A	1121	CLA	NC
15	A	1121	CLA	ND
15	A	1121	CLA	NA
15	A	1135	CLA	NC
15	A	1135	CLA	ND
15	A	1135	CLA	NA
15	A	1101	CLA	NC
15	A	1101	CLA	ND
15	A	1101	CLA	NA
15	1	608	CLA	NC
15	1	608	CLA	ND
15	1	608	CLA	NA
16	2	610	CHL	NC
16	2	610	CHL	ND
16	2	610	CHL	NA
16	2	610	CHL	C3A
15	3	608	CLA	NC
15	3	608	CLA	ND
15	3	608	CLA	NA
15	A	1106	CLA	NC
15	A	1106	CLA	ND
15	A	1106	CLA	NA
15	A	1137	CLA	NC
15	A	1137	CLA	ND
15	A	1137	CLA	NA
15	B	1238	CLA	NC
15	B	1238	CLA	ND
15	B	1238	CLA	NA
15	B	1232	CLA	NC
15	B	1232	CLA	ND
15	B	1232	CLA	NA
15	3	603	CLA	NC
15	3	603	CLA	ND
15	3	603	CLA	NA
15	B	1208	CLA	NC
15	B	1208	CLA	ND
15	B	1208	CLA	NA
15	3	606	CLA	NC
15	3	606	CLA	ND

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Mol	Chain	Res	Type	Atom
15	3	606	CLA	NA
15	A	1131	CLA	NC
15	A	1131	CLA	ND
15	A	1131	CLA	NA
15	A	1125	CLA	NC
15	A	1125	CLA	ND
15	A	1125	CLA	NA
15	A	1105	CLA	NC
15	A	1105	CLA	ND
15	A	1105	CLA	NA
16	1	609	CHL	NC
16	1	609	CHL	ND
16	1	609	CHL	NA
16	1	609	CHL	C3A
15	B	1237	CLA	NC
15	B	1237	CLA	ND
15	B	1237	CLA	NA
15	3	611	CLA	NC
15	3	611	CLA	ND
15	3	611	CLA	NA
15	1	607	CLA	NC
15	1	607	CLA	ND
15	1	607	CLA	NA
15	B	1212	CLA	NC
15	B	1212	CLA	ND
15	B	1212	CLA	NA
16	2	613	CHL	NC
16	2	613	CHL	ND
16	2	613	CHL	NA
15	2	606	CLA	NC
15	2	606	CLA	ND
15	2	606	CLA	NA
15	A	1102	CLA	NC
15	A	1102	CLA	ND
15	A	1102	CLA	NA
24	A	1011	CL0	NC
24	A	1011	CL0	ND
24	A	1011	CL0	NA
15	A	1103	CLA	NC
15	A	1103	CLA	ND
15	A	1103	CLA	NA
15	1	605	CLA	NC

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Mol	Chain	Res	Type	Atom
15	1	605	CLA	ND
15	1	605	CLA	NA
16	4	611	CHL	NC
16	4	611	CHL	ND
16	4	611	CHL	NA

All (1867) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	4	604	CLA	C1A-C2A-CAA-CBA
15	4	604	CLA	C3A-C2A-CAA-CBA
15	4	604	CLA	C2-C1-O2A-CGA
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D
15	4	604	CLA	CAD-CBD-CGD-O1D
15	A	1124	CLA	C1A-C2A-CAA-CBA
15	A	1124	CLA	CBA-CGA-O2A-C1
15	A	1124	CLA	O1A-CGA-O2A-C1
15	A	1124	CLA	CHA-CBD-CGD-O1D
15	A	1124	CLA	CHA-CBD-CGD-O2D
14	B	4001	BCR	C1-C6-C7-C8
14	B	4001	BCR	C5-C6-C7-C8
14	B	4001	BCR	C11-C10-C9-C8
14	B	4001	BCR	C11-C10-C9-C34
14	B	4001	BCR	C10-C11-C12-C13
15	2	608	CLA	CBA-CGA-O2A-C1
15	2	608	CLA	O1A-CGA-O2A-C1
15	2	608	CLA	CHA-CBD-CGD-O1D
15	2	608	CLA	CHA-CBD-CGD-O2D
13	3	502	XAT	C14-C15-C35-C34
13	3	502	XAT	C26-C27-C28-C29
13	3	502	XAT	C27-C28-C29-C30
13	3	502	XAT	C27-C28-C29-C39
13	3	502	XAT	C30-C31-C32-C33
13	3	502	XAT	C32-C33-C34-C35
13	3	502	XAT	C40-C33-C34-C35
15	2	601	CLA	CHA-CBD-CGD-O1D
15	2	601	CLA	CHA-CBD-CGD-O2D
15	2	601	CLA	CAD-CBD-CGD-O1D
15	2	601	CLA	CBD-CGD-O2D-CED
15	B	1218	CLA	C1A-C2A-CAA-CBA
15	B	1218	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	B	1218	CLA	CHA-CBD-CGD-O2D
15	B	1218	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CHA-CBD-CGD-O1D
15	A	1119	CLA	CHA-CBD-CGD-O2D
14	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C11-C10-C9-C34
14	B	4004	BCR	C10-C11-C12-C13
14	B	4004	BCR	C23-C24-C25-C30
15	A	1127	CLA	C1A-C2A-CAA-CBA
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	CHA-CBD-CGD-O1D
15	A	1130	CLA	CHA-CBD-CGD-O2D
14	4	503	BCR	C1-C6-C7-C8
14	4	503	BCR	C5-C6-C7-C8
14	4	503	BCR	C11-C10-C9-C8
14	4	503	BCR	C11-C10-C9-C34
14	4	503	BCR	C10-C11-C12-C13
14	4	503	BCR	C36-C18-C19-C20
14	4	503	BCR	C21-C22-C23-C24
14	4	503	BCR	C37-C22-C23-C24
15	B	1205	CLA	C1A-C2A-CAA-CBA
15	B	1205	CLA	C3A-C2A-CAA-CBA
15	B	1205	CLA	CBD-CGD-O2D-CED
15	A	1013	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	C3A-C2A-CAA-CBA
15	F	1301	CLA	CBD-CGD-O2D-CED
15	B	1213	CLA	CBD-CGD-O2D-CED
14	J	4001	BCR	C5-C6-C7-C8
14	J	4001	BCR	C17-C18-C19-C20
14	J	4001	BCR	C36-C18-C19-C20
14	J	4001	BCR	C23-C24-C25-C26
14	J	4001	BCR	C23-C24-C25-C30
15	3	612	CLA	CHA-CBD-CGD-O1D
15	3	612	CLA	CHA-CBD-CGD-O2D
23	B	5031	GSH	N1-CA1-CB1-CG1
23	B	5031	GSH	C1-CA1-CB1-CG1
23	B	5031	GSH	CA1-CB1-CG1-CD1
23	B	5031	GSH	N2-CA2-CB2-SG2
23	B	5031	GSH	C2-CA2-CB2-SG2
19	1	811	SQD	O5-C5-C6-S
15	1	601	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	1	601	CLA	CHA-CBD-CGD-O1D
15	1	601	CLA	CHA-CBD-CGD-O2D
15	1	601	CLA	CBD-CGD-O2D-CED
15	B	1227	CLA	CBD-CGD-O2D-CED
15	A	1108	CLA	C1A-C2A-CAA-CBA
15	A	1108	CLA	CBD-CGD-O2D-CED
15	B	1214	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	CBD-CGD-O2D-CED
21	4	811	DGD	C2A-C1A-O1G-C1G
21	4	811	DGD	O1A-C1A-O1G-C1G
21	4	811	DGD	C2E-C1E-O5D-C6D
21	4	811	DGD	O6E-C1E-O5D-C6D
15	B	1229	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	CHA-CBD-CGD-O1D
15	B	1229	CLA	CHA-CBD-CGD-O2D
15	B	1229	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	C1A-C2A-CAA-CBA
15	3	607	CLA	C3A-C2A-CAA-CBA
21	B	5002	DGD	C2B-C1B-O2G-C2G
21	B	5002	DGD	O2G-C2G-C3G-O3G
15	B	1209	CLA	CHA-CBD-CGD-O1D
15	B	1209	CLA	CHA-CBD-CGD-O2D
16	4	610	CHL	CHA-CBD-CGD-O1D
16	4	610	CHL	CHA-CBD-CGD-O2D
16	4	610	CHL	CAD-CBD-CGD-O1D
15	4	607	CLA	C1A-C2A-CAA-CBA
15	4	607	CLA	CBD-CGD-O2D-CED
15	B	1204	CLA	C2-C1-O2A-CGA
15	B	1204	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	C1A-C2A-CAA-CBA
15	B	1211	CLA	C3A-C2A-CAA-CBA
15	B	1211	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	C1A-C2A-CAA-CBA
15	A	1109	CLA	C3A-C2A-CAA-CBA
15	A	1113	CLA	C1A-C2A-CAA-CBA
14	J	4003	BCR	C5-C6-C7-C8
14	J	4003	BCR	C11-C10-C9-C8
14	J	4003	BCR	C11-C10-C9-C34
14	J	4003	BCR	C11-C12-C13-C14
14	J	4003	BCR	C11-C12-C13-C35
14	J	4003	BCR	C19-C20-C21-C22
14	J	4003	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	4	608	CLA	CHA-CBD-CGD-O1D
15	4	608	CLA	CHA-CBD-CGD-O2D
15	A	1122	CLA	C1A-C2A-CAA-CBA
15	A	1122	CLA	C3A-C2A-CAA-CBA
15	A	1122	CLA	CBD-CGD-O2D-CED
23	4	831	GSH	C1-CA1-CB1-CG1
15	2	602	CLA	CBD-CGD-O2D-CED
16	4	613	CHL	CHA-CBD-CGD-O1D
16	4	613	CHL	CHA-CBD-CGD-O2D
16	4	613	CHL	CAD-CBD-CGD-O1D
15	2	607	CLA	C1A-C2A-CAA-CBA
15	2	607	CLA	C3A-C2A-CAA-CBA
15	2	607	CLA	CHA-CBD-CGD-O1D
15	2	607	CLA	CHA-CBD-CGD-O2D
15	2	607	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	B	1230	CLA	C2-C1-O2A-CGA
15	B	1230	CLA	CBD-CGD-O2D-CED
14	1	503	BCR	C10-C11-C12-C13
14	1	503	BCR	C17-C18-C19-C20
14	1	503	BCR	C36-C18-C19-C20
14	1	503	BCR	C23-C24-C25-C26
15	3	613	CLA	C1A-C2A-CAA-CBA
15	3	613	CLA	C3A-C2A-CAA-CBA
15	3	613	CLA	CBA-CGA-O2A-C1
15	3	613	CLA	CHA-CBD-CGD-O1D
15	3	613	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CAD-CBD-CGD-O1D
14	J	4002	BCR	C1-C6-C7-C8
14	J	4002	BCR	C5-C6-C7-C8
14	J	4002	BCR	C7-C8-C9-C10
14	J	4002	BCR	C7-C8-C9-C34
14	J	4002	BCR	C11-C10-C9-C8
14	J	4002	BCR	C11-C10-C9-C34
14	J	4002	BCR	C10-C11-C12-C13
14	J	4002	BCR	C17-C18-C19-C20
14	J	4002	BCR	C36-C18-C19-C20
14	J	4002	BCR	C19-C20-C21-C22
14	J	4002	BCR	C37-C22-C23-C24
14	J	4002	BCR	C23-C24-C25-C26
14	J	4002	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
15	2	604	CLA	C2-C1-O2A-CGA
15	2	604	CLA	CBD-CGD-O2D-CED
18	2	803	LMG	C2-C1-O1-C7
18	2	803	LMG	O6-C1-O1-C7
14	B	4006	BCR	C7-C8-C9-C10
14	B	4006	BCR	C7-C8-C9-C34
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C10-C11-C12-C13
14	B	4006	BCR	C17-C18-C19-C20
14	B	4006	BCR	C36-C18-C19-C20
15	A	1138	CLA	C1A-C2A-CAA-CBA
15	A	1138	CLA	C3A-C2A-CAA-CBA
15	J	1302	CLA	C3A-C2A-CAA-CBA
15	J	1302	CLA	CHA-CBD-CGD-O1D
15	J	1302	CLA	CHA-CBD-CGD-O2D
15	B	1231	CLA	CHA-CBD-CGD-O1D
15	B	1231	CLA	CBD-CGD-O2D-CED
14	4	505	BCR	C1-C6-C7-C8
14	4	505	BCR	C5-C6-C7-C8
14	4	505	BCR	C11-C10-C9-C8
14	4	505	BCR	C11-C10-C9-C34
14	4	505	BCR	C11-C12-C13-C35
13	4	502	XAT	C27-C28-C29-C39
15	A	1118	CLA	CHA-CBD-CGD-O1D
15	A	1118	CLA	CHA-CBD-CGD-O2D
15	A	1118	CLA	CAD-CBD-CGD-O1D
15	A	1118	CLA	CAD-CBD-CGD-O2D
15	4	615	CLA	C1A-C2A-CAA-CBA
15	4	615	CLA	C3A-C2A-CAA-CBA
15	4	615	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	C1A-C2A-CAA-CBA
15	A	1129	CLA	C3A-C2A-CAA-CBA
18	2	802	LMG	C2-C1-O1-C7
18	2	802	LMG	O6-C1-O1-C7
18	2	802	LMG	C11-C10-O7-C8
15	B	1215	CLA	C1A-C2A-CAA-CBA
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1215	CLA	CBD-CGD-O2D-CED
15	4	605	CLA	C1A-C2A-CAA-CBA
15	4	605	CLA	C2-C1-O2A-CGA
15	B	1224	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1104	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	CHA-CBD-CGD-O1D
15	A	1104	CLA	CHA-CBD-CGD-O2D
15	2	612	CLA	C1A-C2A-CAA-CBA
15	2	612	CLA	C3A-C2A-CAA-CBA
15	2	612	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	C3A-C2A-CAA-CBA
15	A	1115	CLA	CHA-CBD-CGD-O1D
15	A	1115	CLA	CHA-CBD-CGD-O2D
15	A	1114	CLA	CBA-CGA-O2A-C1
15	A	1114	CLA	CHA-CBD-CGD-O2D
15	3	615	CLA	CBA-CGA-O2A-C1
15	3	615	CLA	CBD-CGD-O2D-CED
14	1	505	BCR	C5-C6-C7-C8
14	1	505	BCR	C11-C10-C9-C8
14	1	505	BCR	C11-C10-C9-C34
14	1	505	BCR	C13-C14-C15-C16
14	1	505	BCR	C19-C20-C21-C22
14	1	505	BCR	C23-C24-C25-C26
15	1	613	CLA	C1A-C2A-CAA-CBA
15	1	613	CLA	C3A-C2A-CAA-CBA
15	1	613	CLA	CBD-CGD-O2D-CED
12	1	501	LUT	C13-C14-C15-C35
12	1	501	LUT	C21-C26-C27-C28
15	B	1220	CLA	C1A-C2A-CAA-CBA
15	B	1220	CLA	C3A-C2A-CAA-CBA
15	B	1220	CLA	CBD-CGD-O2D-CED
18	1	803	LMG	C2-C1-O1-C7
18	1	803	LMG	O6-C1-O1-C7
15	3	610	CLA	C3A-C2A-CAA-CBA
15	A	1123	CLA	C1A-C2A-CAA-CBA
15	A	1123	CLA	CHA-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	CBD-CGD-O2D-CED
15	A	1111	CLA	C1A-C2A-CAA-CBA
15	A	1111	CLA	C3A-C2A-CAA-CBA
15	A	1111	CLA	CHA-CBD-CGD-O1D
15	A	1111	CLA	CHA-CBD-CGD-O2D
17	B	5001	LHG	O1-C1-C2-C3
17	B	5001	LHG	C1-C2-C3-O3
17	B	5001	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O6
17	B	5001	LHG	O6-C4-C5-O7
17	B	5001	LHG	C8-C7-O7-C5
15	4	606	CLA	CHA-CBD-CGD-O1D
15	4	606	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O1D
15	1	602	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	C1A-C2A-CAA-CBA
15	B	1226	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	CHA-CBD-CGD-O1D
15	B	1226	CLA	CHA-CBD-CGD-O2D
15	B	1239	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED
17	1	801	LHG	O2-C2-C3-O3
17	1	801	LHG	C3-O3-P-O5
17	1	801	LHG	C3-O3-P-O6
17	1	801	LHG	C8-C7-O7-C5
15	A	1012	CLA	CBD-CGD-O2D-CED
15	A	1110	CLA	C1A-C2A-CAA-CBA
15	A	1110	CLA	CBD-CGD-O2D-CED
14	2	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C5-C6-C7-C8
14	2	503	BCR	C7-C8-C9-C34
14	2	503	BCR	C11-C10-C9-C8
14	2	503	BCR	C11-C10-C9-C34
14	2	503	BCR	C9-C10-C11-C12
14	2	503	BCR	C10-C11-C12-C13
14	2	503	BCR	C37-C22-C23-C24
14	2	503	BCR	C23-C24-C25-C26
14	2	503	BCR	C23-C24-C25-C30
15	B	1240	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	C3A-C2A-CAA-CBA
15	B	1217	CLA	CAD-CBD-CGD-O1D
15	B	1217	CLA	CAD-CBD-CGD-O2D
21	2	811	DGD	O6D-C1D-O3G-C3G
15	4	602	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	CHA-CBD-CGD-O1D
15	B	1021	CLA	CHA-CBD-CGD-O2D
14	B	4002	BCR	C1-C6-C7-C8
14	B	4002	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	B	4002	BCR	C11-C10-C9-C8
14	B	4002	BCR	C11-C10-C9-C34
14	B	4002	BCR	C10-C11-C12-C13
14	B	4002	BCR	C11-C12-C13-C35
14	B	4002	BCR	C17-C18-C19-C20
14	B	4002	BCR	C36-C18-C19-C20
14	B	4002	BCR	C21-C22-C23-C24
14	B	4002	BCR	C37-C22-C23-C24
21	J	5001	DGD	C2D-C1D-O3G-C3G
21	J	5001	DGD	O6D-C1D-O3G-C3G
15	B	1235	CLA	CHA-CBD-CGD-O1D
15	B	1235	CLA	CHA-CBD-CGD-O2D
15	3	601	CLA	C1A-C2A-CAA-CBA
13	2	502	XAT	O24-C26-C27-C28
15	A	1120	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	C1A-C2A-CAA-CBA
15	A	1141	CLA	C3A-C2A-CAA-CBA
15	B	1228	CLA	CBD-CGD-O2D-CED
16	1	610	CHL	C1A-C2A-CAA-CBA
16	1	610	CHL	C3A-C2A-CAA-CBA
15	2	605	CLA	C1A-C2A-CAA-CBA
15	2	605	CLA	C3A-C2A-CAA-CBA
15	B	1222	CLA	C3A-C2A-CAA-CBA
15	1	612	CLA	C3A-C2A-CAA-CBA
14	F	4002	BCR	C11-C10-C9-C8
14	F	4002	BCR	C11-C10-C9-C34
14	F	4002	BCR	C10-C11-C12-C13
14	F	4002	BCR	C21-C22-C23-C24
14	F	4002	BCR	C37-C22-C23-C24
15	A	1140	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	C2-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
14	A	4005	BCR	C7-C8-C9-C10
17	2	801	LHG	C4-O6-P-O5
17	2	801	LHG	C8-C7-O7-C5
15	B	1023	CLA	C2-C1-O2A-CGA
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	B	1210	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	C3A-C2A-CAA-CBA
15	1	615	CLA	CHA-CBD-CGD-O1D
15	1	615	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	4004	BCR	C23-C24-C25-C26
14	A	4004	BCR	C23-C24-C25-C30
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1116	CLA	C2A-CAA-CBA-CGA
15	A	1116	CLA	O1A-CGA-O2A-C1
14	B	4003	BCR	C11-C10-C9-C8
14	B	4003	BCR	C11-C10-C9-C34
14	B	4003	BCR	C23-C24-C25-C26
14	B	4003	BCR	C23-C24-C25-C30
14	A	4006	BCR	C7-C8-C9-C10
14	A	4006	BCR	C7-C8-C9-C34
14	A	4006	BCR	C11-C12-C13-C35
14	A	4006	BCR	C21-C22-C23-C24
14	A	4006	BCR	C37-C22-C23-C24
14	3	504	BCR	C5-C6-C7-C8
14	3	504	BCR	C11-C10-C9-C8
14	3	504	BCR	C11-C10-C9-C34
14	3	504	BCR	C10-C11-C12-C13
14	3	504	BCR	C11-C12-C13-C35
14	3	503	BCR	C5-C6-C7-C8
14	3	503	BCR	C11-C10-C9-C8
14	3	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C10-C11-C12-C13
14	3	503	BCR	C17-C18-C19-C20
14	3	503	BCR	C36-C18-C19-C20
14	3	503	BCR	C21-C22-C23-C24
14	3	503	BCR	C37-C22-C23-C24
17	A	5001	LHG	O1-C1-C2-C3
17	A	5001	LHG	C1-C2-C3-O3
17	A	5001	LHG	C4-O6-P-O5
17	A	5001	LHG	C4-C5-C6-O8
17	A	5001	LHG	O7-C5-C6-O8
14	A	4007	BCR	C5-C6-C7-C8
14	A	4007	BCR	C11-C10-C9-C8
14	A	4007	BCR	C11-C10-C9-C34
14	A	4007	BCR	C23-C24-C25-C30
15	A	1126	CLA	C2-C1-O2A-CGA
15	2	603	CLA	CHA-CBD-CGD-O1D
15	2	603	CLA	CBD-CGD-O2D-CED
15	A	1139	CLA	C2-C3-C5-C6
15	A	1139	CLA	C4-C3-C5-C6
15	1	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	1	603	CLA	CHA-CBD-CGD-O1D
15	1	603	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	C2-C1-O2A-CGA
15	F	1302	CLA	CHA-CBD-CGD-O1D
15	F	1302	CLA	CHA-CBD-CGD-O2D
15	A	1135	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	A	1101	CLA	CHA-CBD-CGD-O1D
15	A	1101	CLA	CHA-CBD-CGD-O2D
14	A	4003	BCR	C19-C20-C21-C22
14	A	4003	BCR	C21-C22-C23-C24
14	A	4003	BCR	C37-C22-C23-C24
14	A	4003	BCR	C23-C24-C25-C26
15	1	608	CLA	C1A-C2A-CAA-CBA
15	1	608	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1137	CLA	C1A-C2A-CAA-CBA
15	A	1137	CLA	C3A-C2A-CAA-CBA
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D
15	B	1238	CLA	C2-C1-O2A-CGA
17	A	5002	LHG	O1-C1-C2-C3
17	A	5002	LHG	C1-C2-C3-O3
17	A	5002	LHG	O2-C2-C3-O3
17	A	5002	LHG	C8-C7-O7-C5
15	3	603	CLA	C2C-C3C-CAC-CBC
15	3	603	CLA	C4C-C3C-CAC-CBC
15	3	603	CLA	CHA-CBD-CGD-O1D
15	3	603	CLA	CHA-CBD-CGD-O2D
12	2	501	LUT	C7-C8-C9-C19
12	2	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C1-C6-C7-C8
12	4	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C27-C28-C29-C39
15	3	606	CLA	CHA-CBD-CGD-O1D
15	3	606	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	C1A-C2A-CAA-CBA
15	A	1131	CLA	C3A-C2A-CAA-CBA
15	A	1131	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	A	1125	CLA	C1A-C2A-CAA-CBA
15	A	1125	CLA	CHA-CBD-CGD-O1D
15	A	1125	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	C1A-C2A-CAA-CBA
15	A	1105	CLA	C3A-C2A-CAA-CBA
16	1	609	CHL	C1A-C2A-CAA-CBA
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C7-C8-C9-C10
14	B	4005	BCR	C7-C8-C9-C34
14	B	4005	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C34
14	B	4005	BCR	C10-C11-C12-C13
14	B	4005	BCR	C36-C18-C19-C20
12	3	501	LUT	C21-C26-C27-C28
15	B	1237	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C3A-C2A-CAA-CBA
15	3	611	CLA	C2A-CAA-CBA-CGA
15	3	611	CLA	CHA-CBD-CGD-O1D
15	3	611	CLA	CHA-CBD-CGD-O2D
13	1	502	XAT	C30-C31-C32-C33
15	B	1212	CLA	C1A-C2A-CAA-CBA
15	B	1212	CLA	CBD-CGD-O2D-CED
16	2	613	CHL	C2A-CAA-CBA-CGA
15	2	606	CLA	C3A-C2A-CAA-CBA
15	2	606	CLA	C2A-CAA-CBA-CGA
15	2	606	CLA	CBD-CGD-O2D-CED
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1102	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	CBD-CGD-O2D-CED
24	A	1011	CL0	C1A-C2A-CAA-CBA
24	A	1011	CL0	CBD-CGD-O2D-CED
15	A	1103	CLA	C2-C1-O2A-CGA
15	A	1103	CLA	CHA-CBD-CGD-O1D
15	A	1103	CLA	CHA-CBD-CGD-O2D
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	A	1103	CLA	CBD-CGD-O2D-CED
15	1	605	CLA	CBA-CGA-O2A-C1
14	A	4002	BCR	C1-C6-C7-C8
14	A	4002	BCR	C7-C8-C9-C34
14	A	4002	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	A	4002	BCR	C11-C10-C9-C34
14	A	4002	BCR	C11-C12-C13-C14
14	A	4002	BCR	C11-C12-C13-C35
14	A	4002	BCR	C17-C18-C19-C20
14	A	4002	BCR	C36-C18-C19-C20
16	4	611	CHL	CHA-CBD-CGD-O1D
16	4	611	CHL	CHA-CBD-CGD-O2D
16	3	604	CHL	C2C-C3C-CAC-CBC
18	1	803	LMG	C11-C10-O7-C8
15	B	1218	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	O1D-CGD-O2D-CED
15	4	615	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	O1D-CGD-O2D-CED
15	B	1021	CLA	O1D-CGD-O2D-CED
15	2	605	CLA	O1D-CGD-O2D-CED
15	1	612	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	O1D-CGD-O2D-CED
15	A	1139	CLA	O1D-CGD-O2D-CED
18	1	803	LMG	O9-C10-O7-C8
17	B	5001	LHG	O9-C7-O7-C5
17	2	801	LHG	O9-C7-O7-C5
15	2	601	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	B	1224	CLA	O1D-CGD-O2D-CED
15	B	1202	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	O1D-CGD-O2D-CED
15	B	1240	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	1	607	CLA	O1D-CGD-O2D-CED
15	4	604	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	2	608	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	3	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	3	607	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CBD-CGD-O2D-CED
15	A	1136	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	CBD-CGD-O2D-CED
15	A	1113	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	CBD-CGD-O2D-CED
15	A	1118	CLA	CBD-CGD-O2D-CED
15	A	1129	CLA	CBD-CGD-O2D-CED
15	4	605	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	CBD-CGD-O2D-CED
15	A	1104	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	CBD-CGD-O2D-CED
15	3	605	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	B	1022	CLA	CBD-CGD-O2D-CED
15	B	1203	CLA	CBD-CGD-O2D-CED
15	3	610	CLA	CBD-CGD-O2D-CED
15	A	1123	CLA	CBD-CGD-O2D-CED
15	4	606	CLA	CBD-CGD-O2D-CED
15	B	1206	CLA	CBD-CGD-O2D-CED
15	B	1226	CLA	CBD-CGD-O2D-CED
15	A	1132	CLA	CBD-CGD-O2D-CED
15	B	1217	CLA	CBD-CGD-O2D-CED
15	1	606	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	CBD-CGD-O2D-CED
15	4	612	CLA	CBD-CGD-O2D-CED
15	1	611	CLA	CBD-CGD-O2D-CED
15	B	1223	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CBD-CGD-O2D-CED
15	2	605	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	CBD-CGD-O2D-CED
15	1	612	CLA	CBD-CGD-O2D-CED
15	2	615	CLA	CBD-CGD-O2D-CED
15	4	603	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1234	CLA	CBD-CGD-O2D-CED
15	B	1221	CLA	CBD-CGD-O2D-CED
15	B	1219	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1139	CLA	CBD-CGD-O2D-CED
15	B	1201	CLA	CBD-CGD-O2D-CED
15	1	603	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	1	608	CLA	CBD-CGD-O2D-CED
15	3	608	CLA	CBD-CGD-O2D-CED
15	A	1106	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	B	1208	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
15	B	1237	CLA	CBD-CGD-O2D-CED
15	3	611	CLA	CBD-CGD-O2D-CED
15	1	607	CLA	CBD-CGD-O2D-CED
15	1	605	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	O1A-CGA-O2A-C1
15	B	1218	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
15	F	1302	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	O1A-CGA-O2A-C1
15	4	608	CLA	O1A-CGA-O2A-C1
15	1	608	CLA	O1A-CGA-O2A-C1
16	3	604	CHL	C4C-C3C-CAC-CBC
15	A	1124	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	O1D-CGD-O2D-CED
15	A	1119	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	O1D-CGD-O2D-CED
15	A	1117	CLA	O1D-CGD-O2D-CED
15	3	607	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	B	1230	CLA	O1D-CGD-O2D-CED
15	A	1118	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	O1D-CGD-O2D-CED
15	B	1022	CLA	O1D-CGD-O2D-CED
15	3	610	CLA	O1D-CGD-O2D-CED
15	A	1123	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED
15	B	1217	CLA	O1D-CGD-O2D-CED
15	1	611	CLA	O1D-CGD-O2D-CED
15	A	1141	CLA	O1D-CGD-O2D-CED
15	A	1116	CLA	O1D-CGD-O2D-CED
15	B	1234	CLA	O1D-CGD-O2D-CED
15	1	603	CLA	O1D-CGD-O2D-CED
15	B	1225	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	O1D-CGD-O2D-CED
15	B	1232	CLA	O1D-CGD-O2D-CED
15	B	1208	CLA	O1D-CGD-O2D-CED
15	A	1131	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	O1D-CGD-O2D-CED
15	3	611	CLA	O1D-CGD-O2D-CED
24	A	1011	CL0	O1D-CGD-O2D-CED
15	B	1209	CLA	CBA-CGA-O2A-C1
15	4	608	CLA	CBA-CGA-O2A-C1
15	1	608	CLA	CBA-CGA-O2A-C1
15	A	1127	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	O1D-CGD-O2D-CED
15	B	1213	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	B	1214	CLA	O1D-CGD-O2D-CED
15	B	1229	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	4	607	CLA	O1D-CGD-O2D-CED
15	B	1211	CLA	O1D-CGD-O2D-CED
15	A	1109	CLA	O1D-CGD-O2D-CED
15	4	608	CLA	O1D-CGD-O2D-CED
15	2	602	CLA	O1D-CGD-O2D-CED
15	3	613	CLA	O1D-CGD-O2D-CED
15	B	1231	CLA	O1D-CGD-O2D-CED
15	2	612	CLA	O1D-CGD-O2D-CED
15	3	615	CLA	O1D-CGD-O2D-CED
15	B	1220	CLA	O1D-CGD-O2D-CED
15	1	602	CLA	O1D-CGD-O2D-CED
15	B	1239	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1216	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	O1D-CGD-O2D-CED
15	4	602	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	2	615	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	O1D-CGD-O2D-CED
15	B	1210	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	2	603	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	B	1201	CLA	O1D-CGD-O2D-CED
15	F	1302	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	O1D-CGD-O2D-CED
15	B	1238	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	2	606	CLA	O1D-CGD-O2D-CED
15	A	1133	CLA	CBA-CGA-O2A-C1
15	A	1013	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	A	1116	CLA	CBA-CGA-O2A-C1
15	F	1302	CLA	CBA-CGA-O2A-C1
24	A	1011	CL0	CBA-CGA-O2A-C1
15	B	1235	CLA	CBD-CGD-O2D-CED
15	4	609	CLA	CBD-CGD-O2D-CED
15	1	606	CLA	C2C-C3C-CAC-CBC
15	A	1127	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	O1A-CGA-O2A-C1
15	A	1117	CLA	O1A-CGA-O2A-C1
15	A	1136	CLA	O1A-CGA-O2A-C1
15	A	1118	CLA	O1A-CGA-O2A-C1
18	2	802	LMG	O10-C28-O8-C9
15	B	1206	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	O1A-CGA-O2A-C1
15	A	1141	CLA	O1A-CGA-O2A-C1
15	A	1140	CLA	O1A-CGA-O2A-C1
15	1	615	CLA	O1A-CGA-O2A-C1
24	A	1011	CL0	O1A-CGA-O2A-C1
15	A	1114	CLA	O1A-CGA-O2A-C1
15	B	1204	CLA	O1D-CGD-O2D-CED
15	A	1122	CLA	O1D-CGD-O2D-CED
15	2	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1236	CLA	O1D-CGD-O2D-CED
15	A	1120	CLA	O1D-CGD-O2D-CED
15	1	611	CLA	C4C-C3C-CAC-CBC
15	F	1301	CLA	O1D-CGD-O2D-CED
15	A	1108	CLA	O1D-CGD-O2D-CED
15	A	1136	CLA	O1D-CGD-O2D-CED
15	2	604	CLA	O1D-CGD-O2D-CED
15	B	1215	CLA	O1D-CGD-O2D-CED
15	1	613	CLA	O1D-CGD-O2D-CED
15	B	1212	CLA	O1D-CGD-O2D-CED
15	3	601	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	O1D-CGD-O2D-CED
15	2	608	CLA	O1D-CGD-O2D-CED
15	4	612	CLA	O1D-CGD-O2D-CED
15	A	1102	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	O1D-CGD-O2D-CED
21	B	5002	DGD	O1B-C1B-O2G-C2G
18	2	802	LMG	O9-C10-O7-C8
17	1	801	LHG	O9-C7-O7-C5
17	A	5002	LHG	O9-C7-O7-C5
15	B	1217	CLA	CBA-CGA-O2A-C1
15	1	611	CLA	C2C-C3C-CAC-CBC
15	A	1108	CLA	O1A-CGA-O2A-C1
15	B	1209	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	O1A-CGA-O2A-C1
15	A	1130	CLA	C3-C5-C6-C7
15	A	1013	CLA	C3-C5-C6-C7
15	B	1229	CLA	C3-C5-C6-C7
25	B	2002	PQN	C13-C15-C16-C17
15	4	615	CLA	C3-C5-C6-C7
15	B	1220	CLA	C3-C5-C6-C7
25	A	2001	PQN	C13-C15-C16-C17
15	A	1106	CLA	C3-C5-C6-C7
15	B	1218	CLA	CBA-CGA-O2A-C1
15	A	1127	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	C29-C28-O8-C9
15	B	1226	CLA	CBA-CGA-O2A-C1
15	B	1021	CLA	CBA-CGA-O2A-C1
15	A	1120	CLA	CBA-CGA-O2A-C1
15	A	1141	CLA	CBA-CGA-O2A-C1
15	1	615	CLA	CBA-CGA-O2A-C1
15	B	1219	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1126	CLA	CBA-CGA-O2A-C1
19	1	811	SQD	O10-C23-O48-C46
15	A	1128	CLA	O1D-CGD-O2D-CED
15	B	1223	CLA	O1D-CGD-O2D-CED
15	B	1222	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	C2-C1-O2A-CGA
15	4	612	CLA	O1A-CGA-O2A-C1
15	B	1201	CLA	O1A-CGA-O2A-C1
15	3	615	CLA	O1A-CGA-O2A-C1
15	1	606	CLA	C4C-C3C-CAC-CBC
15	A	1108	CLA	CBA-CGA-O2A-C1
15	3	605	CLA	C2C-C3C-CAC-CBC
15	A	1013	CLA	C4-C3-C5-C6
15	2	608	CLA	C2A-CAA-CBA-CGA
15	B	1213	CLA	C2A-CAA-CBA-CGA
15	4	607	CLA	C2A-CAA-CBA-CGA
15	4	612	CLA	C2A-CAA-CBA-CGA
15	B	1201	CLA	C2A-CAA-CBA-CGA
16	2	610	CHL	C2A-CAA-CBA-CGA
15	3	612	CLA	O1D-CGD-O2D-CED
15	A	1115	CLA	O1D-CGD-O2D-CED
15	B	1221	CLA	O1D-CGD-O2D-CED
15	4	604	CLA	CBA-CGA-O2A-C1
15	A	1130	CLA	CBA-CGA-O2A-C1
15	A	1117	CLA	CBA-CGA-O2A-C1
15	4	601	CLA	CBA-CGA-O2A-C1
21	B	5002	DGD	C2A-C1A-O1G-C1G
15	B	1204	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
15	B	1211	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	2	604	CLA	CBA-CGA-O2A-C1
15	A	1118	CLA	CBA-CGA-O2A-C1
15	4	606	CLA	CBA-CGA-O2A-C1
15	B	1206	CLA	CBA-CGA-O2A-C1
15	3	601	CLA	CBA-CGA-O2A-C1
15	A	1140	CLA	CBA-CGA-O2A-C1
15	B	1232	CLA	CBA-CGA-O2A-C1
19	1	811	SQD	C24-C23-O48-C46
15	1	604	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	1	608	CLA	O1D-CGD-O2D-CED
15	4	601	CLA	CBD-CGD-O2D-CED
24	A	1011	CL0	C2C-C3C-CAC-CBC
15	A	1104	CLA	O1D-CGD-O2D-CED
15	3	605	CLA	O1D-CGD-O2D-CED
15	B	1226	CLA	O1D-CGD-O2D-CED
15	1	606	CLA	O1D-CGD-O2D-CED
15	1	615	CLA	O1D-CGD-O2D-CED
15	A	1101	CLA	O1D-CGD-O2D-CED
15	A	1106	CLA	O1D-CGD-O2D-CED
15	3	612	CLA	O1A-CGA-O2A-C1
15	4	601	CLA	O1A-CGA-O2A-C1
21	B	5002	DGD	O1A-C1A-O1G-C1G
15	B	1204	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	O1A-CGA-O2A-C1
15	B	1216	CLA	O1A-CGA-O2A-C1
15	3	601	CLA	O1A-CGA-O2A-C1
15	A	1120	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	O1A-CGA-O2A-C1
15	B	1208	CLA	O1A-CGA-O2A-C1
18	1	803	LMG	O10-C28-O8-C9
18	1	803	LMG	C29-C28-O8-C9
15	3	606	CLA	C2A-CAA-CBA-CGA
15	3	613	CLA	O1A-CGA-O2A-C1
13	3	502	XAT	C33-C34-C35-C15
14	F	4002	BCR	C9-C10-C11-C12
14	A	4005	BCR	C13-C14-C15-C16
14	3	503	BCR	C9-C10-C11-C12
17	B	5001	LHG	O2-C2-C3-O3
17	A	5001	LHG	O2-C2-C3-O3
15	A	1119	CLA	CBA-CGA-O2A-C1
15	3	612	CLA	CBA-CGA-O2A-C1
15	4	615	CLA	CBA-CGA-O2A-C1
15	B	1215	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	CBA-CGA-O2A-C1
15	B	1216	CLA	CBA-CGA-O2A-C1
15	A	1132	CLA	CBA-CGA-O2A-C1
15	4	612	CLA	CBA-CGA-O2A-C1
15	2	615	CLA	CBA-CGA-O2A-C1
15	B	1201	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1126	CLA	O1A-CGA-O2A-C1
15	A	1134	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	O1D-CGD-O2D-CED
15	1	607	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	C3-C5-C6-C7
15	B	1208	CLA	CBA-CGA-O2A-C1
15	4	604	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1A-CGA-O2A-C1
15	B	1230	CLA	O1A-CGA-O2A-C1
15	2	604	CLA	O1A-CGA-O2A-C1
15	B	1202	CLA	O1A-CGA-O2A-C1
15	B	1240	CLA	C4-C3-C5-C6
25	A	2001	PQN	C14-C13-C15-C16
15	B	1240	CLA	C2-C3-C5-C6
25	A	2001	PQN	C12-C13-C15-C16
15	J	1302	CLA	C2A-CAA-CBA-CGA
15	2	612	CLA	C2A-CAA-CBA-CGA
15	4	606	CLA	C2A-CAA-CBA-CGA
15	1	611	CLA	C2A-CAA-CBA-CGA
15	F	1302	CLA	C2A-CAA-CBA-CGA
15	4	605	CLA	O1D-CGD-O2D-CED
15	B	1211	CLA	O1A-CGA-O2A-C1
15	4	606	CLA	O1A-CGA-O2A-C1
15	A	1132	CLA	O1A-CGA-O2A-C1
19	1	811	SQD	O5-C1-O6-C44
15	B	1231	CLA	CBA-CGA-O2A-C1
15	B	1220	CLA	CBA-CGA-O2A-C1
15	A	1107	CLA	CBA-CGA-O2A-C1
15	3	611	CLA	CBA-CGA-O2A-C1
15	3	605	CLA	C4C-C3C-CAC-CBC
15	B	1235	CLA	O1D-CGD-O2D-CED
15	4	615	CLA	O1A-CGA-O2A-C1
15	B	1215	CLA	O1A-CGA-O2A-C1
15	2	615	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C1-C2-C3-O3
15	B	1231	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	CBA-CGA-O2A-C1
15	A	1122	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	B	1239	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	2	605	CLA	CBA-CGA-O2A-C1
15	B	1222	CLA	CBA-CGA-O2A-C1
15	B	1210	CLA	CBA-CGA-O2A-C1
15	A	1112	CLA	CBA-CGA-O2A-C1
15	A	1135	CLA	CBA-CGA-O2A-C1
15	B	1238	CLA	CBA-CGA-O2A-C1
15	A	1131	CLA	CBA-CGA-O2A-C1
15	A	1102	CLA	C2A-CAA-CBA-CGA
14	B	4001	BCR	C9-C10-C11-C12
14	4	503	BCR	C9-C10-C11-C12
14	J	4001	BCR	C19-C20-C21-C22
14	1	503	BCR	C13-C14-C15-C16
14	J	4002	BCR	C9-C10-C11-C12
14	B	4003	BCR	C19-C20-C21-C22
14	A	4007	BCR	C19-C20-C21-C22
16	4	611	CHL	C2C-C3C-CAC-CBC
25	A	2001	PQN	C20-C21-C22-C23
15	2	605	CLA	C5-C6-C7-C8
21	4	811	DGD	C2D-C1D-O3G-C3G
15	B	1229	CLA	O1A-CGA-O2A-C1
15	B	1239	CLA	O1A-CGA-O2A-C1
15	B	1222	CLA	O1A-CGA-O2A-C1
15	A	1135	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	C11-C12-C13-C14
25	B	2002	PQN	C19-C18-C20-C21
15	A	1012	CLA	C11-C10-C8-C9
25	A	2001	PQN	C19-C18-C20-C21
15	A	1106	CLA	C11-C12-C13-C14
15	4	609	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	C5-C6-C7-C8
16	3	604	CHL	C2A-CAA-CBA-CGA
15	2	604	CLA	C2A-CAA-CBA-CGA
15	A	1105	CLA	C2A-CAA-CBA-CGA
14	B	4001	BCR	C7-C8-C9-C34
14	B	4001	BCR	C36-C18-C19-C20
14	B	4004	BCR	C36-C18-C19-C20
14	J	4001	BCR	C7-C8-C9-C34
14	J	4003	BCR	C7-C8-C9-C34
14	1	503	BCR	C7-C8-C9-C34
14	B	4006	BCR	C37-C22-C23-C24
14	4	505	BCR	C36-C18-C19-C20
13	2	502	XAT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
14	F	4002	BCR	C36-C18-C19-C20
14	A	4004	BCR	C36-C18-C19-C20
14	A	4006	BCR	C36-C18-C19-C20
14	3	503	BCR	C11-C12-C13-C35
14	A	4003	BCR	C36-C18-C19-C20
14	B	4005	BCR	C37-C22-C23-C24
14	B	4001	BCR	C17-C18-C19-C20
14	J	4001	BCR	C7-C8-C9-C10
14	J	4002	BCR	C21-C22-C23-C24
14	B	4006	BCR	C21-C22-C23-C24
14	4	505	BCR	C17-C18-C19-C20
14	2	503	BCR	C7-C8-C9-C10
14	F	4002	BCR	C17-C18-C19-C20
14	A	4004	BCR	C17-C18-C19-C20
14	A	4006	BCR	C17-C18-C19-C20
18	1	802	LMG	C11-C10-O7-C8
15	A	1122	CLA	O1A-CGA-O2A-C1
15	2	605	CLA	O1A-CGA-O2A-C1
15	B	1210	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	C13-C15-C16-C17
24	A	1011	CL0	C4C-C3C-CAC-CBC
15	F	1301	CLA	CBA-CGA-O2A-C1
15	J	1302	CLA	CBA-CGA-O2A-C1
21	2	811	DGD	C2A-C1A-O1G-C1G
15	A	1013	CLA	C5-C6-C7-C8
15	B	1021	CLA	C8-C10-C11-C12
15	B	1021	CLA	C13-C15-C16-C17
15	2	605	CLA	C13-C15-C16-C17
15	1	612	CLA	C5-C6-C7-C8
15	A	1106	CLA	C5-C6-C7-C8
15	A	1106	CLA	C8-C10-C11-C12
15	B	1238	CLA	O1A-CGA-O2A-C1
25	A	2001	PQN	C15-C16-C17-C18
15	B	1225	CLA	CBA-CGA-O2A-C1
15	A	1133	CLA	C2-C1-O2A-CGA
15	A	1119	CLA	C2-C1-O2A-CGA
15	A	1134	CLA	C2-C1-O2A-CGA
15	B	1205	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	C2-C1-O2A-CGA
15	3	612	CLA	C2-C1-O2A-CGA
15	3	607	CLA	C2-C1-O2A-CGA
15	4	607	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	A	1136	CLA	C2-C1-O2A-CGA
15	A	1109	CLA	C2-C1-O2A-CGA
15	A	1122	CLA	C2-C1-O2A-CGA
15	2	602	CLA	C2-C1-O2A-CGA
15	2	607	CLA	C2-C1-O2A-CGA
15	A	1128	CLA	C2-C1-O2A-CGA
15	J	1302	CLA	C2-C1-O2A-CGA
15	B	1231	CLA	C2-C1-O2A-CGA
15	A	1129	CLA	C2-C1-O2A-CGA
15	B	1224	CLA	C2-C1-O2A-CGA
15	B	1202	CLA	C2-C1-O2A-CGA
15	2	612	CLA	C2-C1-O2A-CGA
15	A	1115	CLA	C2-C1-O2A-CGA
15	B	1203	CLA	C2-C1-O2A-CGA
15	B	1220	CLA	C2-C1-O2A-CGA
15	3	610	CLA	C2-C1-O2A-CGA
15	B	1236	CLA	C2-C1-O2A-CGA
15	4	606	CLA	C2-C1-O2A-CGA
15	B	1206	CLA	C2-C1-O2A-CGA
15	B	1226	CLA	C2-C1-O2A-CGA
15	B	1239	CLA	C2-C1-O2A-CGA
15	A	1132	CLA	C2-C1-O2A-CGA
15	B	1021	CLA	C2-C1-O2A-CGA
15	A	1141	CLA	C2-C1-O2A-CGA
15	2	615	CLA	C2-C1-O2A-CGA
15	B	1210	CLA	C2-C1-O2A-CGA
15	B	1234	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
15	A	1112	CLA	C2-C1-O2A-CGA
15	A	1139	CLA	C2-C1-O2A-CGA
15	B	1201	CLA	C2-C1-O2A-CGA
15	B	1225	CLA	C2-C1-O2A-CGA
15	A	1121	CLA	C2-C1-O2A-CGA
15	A	1135	CLA	C2-C1-O2A-CGA
15	3	608	CLA	C2-C1-O2A-CGA
15	A	1125	CLA	C2-C1-O2A-CGA
15	B	1237	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	C12-C13-C15-C16
15	A	1106	CLA	C11-C12-C13-C15
15	3	612	CLA	C3-C5-C6-C7
15	B	1235	CLA	O1A-CGA-O2A-C1
15	A	1112	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1131	CLA	O1A-CGA-O2A-C1
13	3	502	XAT	C29-C30-C31-C32
14	B	4004	BCR	C9-C10-C11-C12
14	1	503	BCR	C15-C16-C17-C18
14	J	4002	BCR	C13-C14-C15-C16
14	4	505	BCR	C13-C14-C15-C16
14	A	4005	BCR	C19-C20-C21-C22
15	A	1130	CLA	C2A-CAA-CBA-CGA
15	A	1129	CLA	C2A-CAA-CBA-CGA
15	B	1022	CLA	C2A-CAA-CBA-CGA
15	B	1234	CLA	C2A-CAA-CBA-CGA
15	A	1121	CLA	C2A-CAA-CBA-CGA
15	3	601	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	C5-C6-C7-C8
15	B	1220	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	O1A-CGA-O2A-C1
21	4	811	DGD	O6D-C1D-O3G-C3G
25	A	2001	PQN	C23-C25-C26-C27
13	4	502	XAT	C10-C11-C12-C13
14	A	4006	BCR	C10-C11-C12-C13
14	A	4007	BCR	C10-C11-C12-C13
14	A	4003	BCR	C10-C11-C12-C13
13	1	502	XAT	C10-C11-C12-C13
21	2	811	DGD	C8A-C9A-CAA-CBA
17	2	801	LHG	O2-C2-C3-O3
15	1	607	CLA	O1A-CGA-O2A-C1
25	A	2001	PQN	C25-C26-C27-C28
15	A	1107	CLA	O1A-CGA-O2A-C1
15	B	1228	CLA	O1A-CGA-O2A-C1
15	F	1301	CLA	O1A-CGA-O2A-C1
15	J	1302	CLA	O1A-CGA-O2A-C1
21	J	5001	DGD	C4D-C5D-C6D-O5D
15	A	1013	CLA	C15-C16-C17-C18
25	A	2001	PQN	C18-C20-C21-C22
15	B	1225	CLA	O1A-CGA-O2A-C1
16	4	611	CHL	C4C-C3C-CAC-CBC
17	2	801	LHG	C1-C2-C3-O3
18	1	802	LMG	O9-C10-O7-C8
15	A	1013	CLA	C2-C3-C5-C6
15	B	1240	CLA	C13-C15-C16-C17
15	A	1117	CLA	C2A-CAA-CBA-CGA
15	F	1301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1215	CLA	C2A-CAA-CBA-CGA
15	3	601	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	B	1208	CLA	C2A-CAA-CBA-CGA
15	A	1128	CLA	CBA-CGA-O2A-C1
15	4	605	CLA	CBA-CGA-O2A-C1
15	3	608	CLA	CBA-CGA-O2A-C1
15	B	1212	CLA	C2A-CAA-CBA-CGA
13	3	502	XAT	C20-C13-C14-C15
14	J	4001	BCR	C11-C10-C9-C34
14	1	503	BCR	C11-C10-C9-C34
13	4	502	XAT	C20-C13-C14-C15
14	A	4005	BCR	C11-C10-C9-C34
14	A	4006	BCR	C11-C10-C9-C34
14	A	4003	BCR	C11-C10-C9-C34
21	2	811	DGD	O1A-C1A-O1G-C1G
15	3	612	CLA	C6-C7-C8-C10
15	B	1235	CLA	C11-C12-C13-C15
15	2	605	CLA	C16-C17-C18-C19
15	3	607	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C6-C5-O7-C7
15	4	601	CLA	O1D-CGD-O2D-CED
15	A	1110	CLA	C2C-C3C-CAC-CBC
13	3	502	XAT	C12-C13-C14-C15
14	J	4001	BCR	C11-C10-C9-C8
14	1	503	BCR	C11-C10-C9-C8
13	4	502	XAT	C12-C13-C14-C15
21	2	811	DGD	C2D-C1D-O3G-C3G
14	A	4006	BCR	C11-C10-C9-C8
14	A	4003	BCR	C11-C10-C9-C8
15	A	1138	CLA	C16-C17-C18-C19
15	A	1103	CLA	C6-C7-C8-C9
15	A	1138	CLA	C11-C10-C8-C9
15	A	1104	CLA	C5-C6-C7-C8
15	1	615	CLA	C8-C10-C11-C12
15	A	1013	CLA	C2A-CAA-CBA-CGA
15	A	1136	CLA	C2A-CAA-CBA-CGA
15	A	1138	CLA	C2A-CAA-CBA-CGA
15	A	1118	CLA	C2A-CAA-CBA-CGA
15	1	602	CLA	C2A-CAA-CBA-CGA
16	1	610	CHL	C2A-CAA-CBA-CGA
24	A	1011	CL0	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	1	605	CLA	C2A-CAA-CBA-CGA
14	3	504	BCR	C7-C8-C9-C34
14	3	504	BCR	C36-C18-C19-C20
16	1	610	CHL	C2C-C3C-CAC-CBC
17	1	801	LHG	O1-C1-C2-C3
17	2	801	LHG	O1-C1-C2-C3
14	B	4001	BCR	C7-C8-C9-C10
14	4	505	BCR	C11-C12-C13-C14
14	2	503	BCR	C21-C22-C23-C24
14	A	4006	BCR	C11-C12-C13-C14
14	3	504	BCR	C11-C12-C13-C14
12	2	501	LUT	C7-C8-C9-C10
14	B	4005	BCR	C17-C18-C19-C20
15	B	1240	CLA	C16-C17-C18-C19
15	B	1240	CLA	C16-C17-C18-C20
15	B	1023	CLA	C11-C12-C13-C14
15	B	1023	CLA	C11-C12-C13-C15
15	A	1103	CLA	C6-C7-C8-C10
15	1	602	CLA	CBA-CGA-O2A-C1
15	A	1128	CLA	O1A-CGA-O2A-C1
15	3	608	CLA	O1A-CGA-O2A-C1
15	3	611	CLA	O1A-CGA-O2A-C1
21	J	5001	DGD	O6D-C5D-C6D-O5D
15	A	1124	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	4	607	CLA	C3A-C2A-CAA-CBA
15	A	1123	CLA	C3A-C2A-CAA-CBA
15	B	1206	CLA	C3A-C2A-CAA-CBA
15	1	602	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C3A-C2A-CAA-CBA
15	3	601	CLA	C3A-C2A-CAA-CBA
15	B	1223	CLA	C3A-C2A-CAA-CBA
15	2	615	CLA	C3A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	B	1234	CLA	C3A-C2A-CAA-CBA
15	B	1221	CLA	C3A-C2A-CAA-CBA
15	1	603	CLA	C3A-C2A-CAA-CBA
15	A	1135	CLA	C3A-C2A-CAA-CBA
15	3	608	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
16	1	609	CHL	C3A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1138	CLA	C16-C17-C18-C20
15	A	1104	CLA	C11-C12-C13-C15
15	2	605	CLA	C16-C17-C18-C20
15	A	1130	CLA	C4-C3-C5-C6
15	A	1130	CLA	C2-C3-C5-C6
21	2	811	DGD	C2G-C1G-O1G-C1A
17	1	801	LHG	O1-C1-C2-O2
17	2	801	LHG	O1-C1-C2-O2
17	A	5001	LHG	O1-C1-C2-O2
22	2	821	LMT	O5'-C5'-C6'-O6'
15	B	1235	CLA	C11-C12-C13-C14
16	2	609	CHL	C2C-C3C-CAC-CBC
18	1	802	LMG	C33-C34-C35-C36
15	A	1130	CLA	C2-C1-O2A-CGA
15	B	1213	CLA	C2-C1-O2A-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1022	CLA	C2-C1-O2A-CGA
15	A	1123	CLA	C2-C1-O2A-CGA
15	A	1111	CLA	C2-C1-O2A-CGA
15	B	1216	CLA	C2-C1-O2A-CGA
15	1	611	CLA	C2-C1-O2A-CGA
15	B	1223	CLA	C2-C1-O2A-CGA
15	A	1120	CLA	C2-C1-O2A-CGA
15	B	1228	CLA	C2-C1-O2A-CGA
15	2	605	CLA	C2-C1-O2A-CGA
15	B	1222	CLA	C2-C1-O2A-CGA
15	A	1140	CLA	C2-C1-O2A-CGA
15	1	615	CLA	C2-C1-O2A-CGA
15	A	1116	CLA	C2-C1-O2A-CGA
15	B	1219	CLA	C2-C1-O2A-CGA
15	A	1137	CLA	C2-C1-O2A-CGA
15	B	1208	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	C2-C1-O2A-CGA
15	4	605	CLA	O1A-CGA-O2A-C1
14	B	4001	BCR	C23-C24-C25-C30
14	B	4004	BCR	C23-C24-C25-C26
14	J	4001	BCR	C1-C6-C7-C8
14	J	4003	BCR	C1-C6-C7-C8
14	J	4003	BCR	C23-C24-C25-C30
14	1	503	BCR	C1-C6-C7-C8
14	1	503	BCR	C5-C6-C7-C8
14	1	503	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
14	4	505	BCR	C23-C24-C25-C26
14	4	505	BCR	C23-C24-C25-C30
14	1	505	BCR	C1-C6-C7-C8
14	1	505	BCR	C23-C24-C25-C30
15	B	1021	CLA	C3-C5-C6-C7
14	B	4003	BCR	C1-C6-C7-C8
14	B	4003	BCR	C5-C6-C7-C8
14	3	504	BCR	C1-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C26
14	3	504	BCR	C23-C24-C25-C30
14	3	503	BCR	C1-C6-C7-C8
14	A	4007	BCR	C1-C6-C7-C8
14	A	4007	BCR	C23-C24-C25-C26
14	A	4003	BCR	C23-C24-C25-C30
12	4	501	LUT	C5-C6-C7-C8
14	B	4005	BCR	C23-C24-C25-C26
14	B	4005	BCR	C23-C24-C25-C30
14	A	4002	BCR	C5-C6-C7-C8
15	B	1205	CLA	CBA-CGA-O2A-C1
15	1	604	CLA	CBA-CGA-O2A-C1
15	2	612	CLA	CBA-CGA-O2A-C1
15	4	609	CLA	CBA-CGA-O2A-C1
15	B	1235	CLA	C10-C11-C12-C13
15	3	607	CLA	O1A-CGA-O2A-C1
15	B	1235	CLA	C4-C3-C5-C6
15	A	1138	CLA	C11-C10-C8-C7
15	4	609	CLA	O1A-CGA-O2A-C1
18	2	802	LMG	O7-C10-C11-C12
15	B	1229	CLA	C10-C11-C12-C13
14	B	4004	BCR	C19-C20-C21-C22
14	4	503	BCR	C19-C20-C21-C22
14	A	4005	BCR	C9-C10-C11-C12
14	3	503	BCR	C19-C20-C21-C22
15	A	1121	CLA	CBA-CGA-O2A-C1
15	B	1211	CLA	C2A-CAA-CBA-CGA
15	A	1115	CLA	C2A-CAA-CBA-CGA
16	2	609	CHL	C2A-CAA-CBA-CGA
15	A	1140	CLA	C2A-CAA-CBA-CGA
15	1	607	CLA	C2A-CAA-CBA-CGA
15	A	1013	CLA	C13-C15-C16-C17
19	1	811	SQD	C14-C15-C16-C17
15	B	1220	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	2	605	CLA	C15-C16-C17-C18
15	B	1239	CLA	C3-C5-C6-C7
15	A	1012	CLA	C3-C5-C6-C7
15	A	1134	CLA	CBA-CGA-O2A-C1
15	B	1205	CLA	O1A-CGA-O2A-C1
15	2	612	CLA	O1A-CGA-O2A-C1
15	A	1138	CLA	C13-C15-C16-C17
15	B	1235	CLA	C2-C3-C5-C6
15	A	1013	CLA	C11-C10-C8-C9
15	B	1235	CLA	C2A-CAA-CBA-CGA
15	1	612	CLA	C2A-CAA-CBA-CGA
15	A	1135	CLA	C2A-CAA-CBA-CGA
18	2	803	LMG	O6-C5-C6-O5
14	1	503	BCR	C37-C22-C23-C24
12	2	501	LUT	C31-C32-C33-C40
15	1	604	CLA	O1A-CGA-O2A-C1
15	2	608	CLA	C1A-C2A-CAA-CBA
15	2	601	CLA	C1A-C2A-CAA-CBA
15	F	1301	CLA	C1A-C2A-CAA-CBA
15	1	601	CLA	C1A-C2A-CAA-CBA
15	B	1204	CLA	C1A-C2A-CAA-CBA
15	2	604	CLA	C1A-C2A-CAA-CBA
15	J	1302	CLA	C1A-C2A-CAA-CBA
15	A	1118	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	A	1115	CLA	C1A-C2A-CAA-CBA
15	3	610	CLA	C1A-C2A-CAA-CBA
15	1	602	CLA	C1A-C2A-CAA-CBA
15	B	1239	CLA	C1A-C2A-CAA-CBA
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	B	1217	CLA	C1A-C2A-CAA-CBA
15	1	606	CLA	C1A-C2A-CAA-CBA
15	B	1021	CLA	C1A-C2A-CAA-CBA
15	B	1223	CLA	C1A-C2A-CAA-CBA
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	B	1222	CLA	C1A-C2A-CAA-CBA
15	1	612	CLA	C1A-C2A-CAA-CBA
15	2	615	CLA	C1A-C2A-CAA-CBA
15	1	615	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	B	1221	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	1219	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1135	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	B	1208	CLA	C1A-C2A-CAA-CBA
15	2	606	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
25	B	2002	PQN	C26-C27-C28-C30
15	A	1104	CLA	C11-C12-C13-C14
14	4	505	BCR	C19-C20-C21-C22
14	2	503	BCR	C19-C20-C21-C22
14	A	4004	BCR	C19-C20-C21-C22
14	3	504	BCR	C9-C10-C11-C12
17	A	5001	LHG	C4-O6-P-O3
15	B	1240	CLA	C3-C5-C6-C7
15	B	1239	CLA	C13-C15-C16-C17
15	3	612	CLA	C6-C7-C8-C9
15	A	1104	CLA	C8-C10-C11-C12
15	A	1121	CLA	O1A-CGA-O2A-C1
21	B	5002	DGD	C1G-C2G-C3G-O3G
15	A	1103	CLA	CBA-CGA-O2A-C1
21	4	811	DGD	C5D-C6D-O5D-C1E
21	2	811	DGD	C2G-C3G-O3G-C1D
21	4	811	DGD	O6E-C5E-C6E-O5E
15	B	1220	CLA	CAA-CBA-CGA-O2A
18	1	802	LMG	O6-C5-C6-O5
17	B	5001	LHG	O1-C1-C2-O2
17	A	5002	LHG	O1-C1-C2-O2
14	B	4005	BCR	C13-C14-C15-C16
21	J	5001	DGD	O6E-C5E-C6E-O5E
15	A	1104	CLA	C4-C3-C5-C6
15	3	601	CLA	C2C-C3C-CAC-CBC
15	B	1224	CLA	C2A-CAA-CBA-CGA
15	A	1126	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	C15-C16-C17-C18
15	2	608	CLA	C2-C1-O2A-CGA
15	A	1127	CLA	C2-C1-O2A-CGA
15	B	1214	CLA	C2-C1-O2A-CGA
15	4	601	CLA	C2-C1-O2A-CGA
15	A	1118	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	4	612	CLA	C2-C1-O2A-CGA
15	4	609	CLA	C2-C1-O2A-CGA
15	B	1232	CLA	C2-C1-O2A-CGA
15	1	601	CLA	CBA-CGA-O2A-C1
15	A	1134	CLA	O1A-CGA-O2A-C1
18	1	802	LMG	C2-C1-O1-C7
18	1	802	LMG	O1-C7-C8-O7
15	B	1229	CLA	C4-C3-C5-C6
15	A	1104	CLA	C2-C3-C5-C6
15	A	1012	CLA	C6-C7-C8-C10
15	B	1240	CLA	C12-C13-C15-C16
25	A	2001	PQN	C21-C22-C23-C25
15	1	615	CLA	C11-C10-C8-C7
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	B	1023	CLA	C11-C10-C8-C9
15	B	1229	CLA	C5-C6-C7-C8
15	3	606	CLA	C2C-C3C-CAC-CBC
14	1	503	BCR	C7-C8-C9-C10
14	1	503	BCR	C21-C22-C23-C24
13	4	502	XAT	C27-C28-C29-C30
14	3	503	BCR	C11-C12-C13-C14
14	A	4002	BCR	C7-C8-C9-C10
15	B	1236	CLA	CBA-CGA-O2A-C1
15	B	1023	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C26-C27-C28-C29
17	B	5001	LHG	O6-C4-C5-C6
17	A	5002	LHG	O6-C4-C5-C6
15	B	1203	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C20-C21-C22-C23
15	2	607	CLA	CBA-CGA-O2A-C1
15	A	1012	CLA	CBA-CGA-O2A-C1
15	B	1237	CLA	CAA-CBA-CGA-O2A
21	4	811	DGD	C2B-C3B-C4B-C5B
15	A	1118	CLA	C3A-C2A-CAA-CBA
15	B	1239	CLA	C3A-C2A-CAA-CBA
15	A	1140	CLA	C3A-C2A-CAA-CBA
15	A	1125	CLA	C3A-C2A-CAA-CBA
15	1	607	CLA	C3A-C2A-CAA-CBA
24	A	1011	CL0	C3A-C2A-CAA-CBA
14	A	4006	BCR	C19-C20-C21-C22
14	B	4005	BCR	C9-C10-C11-C12
23	B	5031	GSH	OE1-CD1-CG1-CB1

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Mol	Chain	Res	Type	Atoms
21	2	811	DGD	O1G-C1G-C2G-C3G
18	1	802	LMG	O1-C7-C8-C9
15	A	1103	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	C2-C3-C5-C6
17	B	5001	LHG	C4-O6-P-O3
15	1	602	CLA	O1A-CGA-O2A-C1
15	4	615	CLA	C5-C6-C7-C8
17	A	5001	LHG	O6-C4-C5-O7
17	A	5002	LHG	O6-C4-C5-O7
15	1	601	CLA	O1A-CGA-O2A-C1
15	3	603	CLA	C2A-CAA-CBA-CGA
15	2	604	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	O1A-CGA-O2A-C1
21	4	811	DGD	O2G-C2G-C3G-O3G
15	A	1129	CLA	CBA-CGA-O2A-C1
15	A	1108	CLA	C2C-C3C-CAC-CBC
15	A	1013	CLA	C14-C13-C15-C16
15	B	1239	CLA	C14-C13-C15-C16
15	B	1235	CLA	C11-C10-C8-C9
25	A	2001	PQN	C21-C22-C23-C24
15	B	1231	CLA	C10-C11-C12-C13
17	1	801	LHG	C2-C3-O3-P
12	1	501	LUT	C1-C6-C7-C8
12	1	501	LUT	C5-C6-C7-C8
14	F	4002	BCR	C1-C6-C7-C8
14	A	4005	BCR	C1-C6-C7-C8
14	A	4005	BCR	C5-C6-C7-C8
15	1	615	CLA	C3-C5-C6-C7
14	A	4002	BCR	C23-C24-C25-C26
14	A	4002	BCR	C23-C24-C25-C30
21	2	811	DGD	O1G-C1A-C2A-C3A
15	1	607	CLA	CAA-CBA-CGA-O2A
14	B	4004	BCR	C17-C18-C19-C20
14	4	503	BCR	C17-C18-C19-C20
14	J	4003	BCR	C7-C8-C9-C10
14	B	4002	BCR	C11-C12-C13-C14
14	A	4003	BCR	C17-C18-C19-C20
12	2	501	LUT	C31-C32-C33-C34
12	4	501	LUT	C27-C28-C29-C30
14	B	4005	BCR	C21-C22-C23-C24
15	B	1240	CLA	C10-C11-C12-C13
15	A	1110	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	C4-C5-O7-C7
17	A	5001	LHG	C6-C5-O7-C7
15	B	1229	CLA	C12-C13-C15-C16
15	A	1104	CLA	C11-C10-C8-C7
15	B	1235	CLA	C11-C10-C8-C7
15	B	1023	CLA	C11-C10-C8-C7
14	B	4006	BCR	C9-C10-C11-C12
14	3	504	BCR	C19-C20-C21-C22
12	4	501	LUT	C29-C30-C31-C32
14	B	4005	BCR	C19-C20-C21-C22
15	2	601	CLA	CBA-CGA-O2A-C1
23	B	5031	GSH	N2-CD1-CG1-CB1
15	B	1239	CLA	C10-C11-C12-C13
15	A	1106	CLA	CBA-CGA-O2A-C1
25	B	2002	PQN	C18-C20-C21-C22
15	2	601	CLA	CAD-CBD-CGD-O2D
15	B	1227	CLA	CAD-CBD-CGD-O2D
16	4	610	CHL	CAD-CBD-CGD-O2D
15	4	607	CLA	CAD-CBD-CGD-O2D
15	B	1204	CLA	CAD-CBD-CGD-O2D
16	4	613	CHL	CAD-CBD-CGD-O2D
15	1	604	CLA	CAD-CBD-CGD-O2D
15	B	1224	CLA	CAD-CBD-CGD-O2D
15	A	1121	CLA	CAD-CBD-CGD-O2D
15	B	1239	CLA	C15-C16-C17-C18
15	1	612	CLA	C14-C13-C15-C16
21	4	811	DGD	O1G-C1G-C2G-C3G
21	4	811	DGD	C1G-C2G-C3G-O3G
17	A	5002	LHG	C4-C5-C6-O8
15	A	1129	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	C5-C6-C7-C8
14	B	4003	BCR	C18-C19-C20-C21
15	B	1214	CLA	O2A-C1-C2-C3
15	4	602	CLA	O2A-C1-C2-C3
15	A	1108	CLA	CHA-CBD-CGD-O1D
15	A	1108	CLA	CHA-CBD-CGD-O2D
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	A	1122	CLA	CHA-CBD-CGD-O1D
15	3	613	CLA	CHA-CBD-CGD-O2D
15	A	1138	CLA	CHA-CBD-CGD-O1D
15	A	1138	CLA	CHA-CBD-CGD-O2D
15	B	1231	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	1129	CLA	CHA-CBD-CGD-O1D
15	A	1129	CLA	CHA-CBD-CGD-O2D
15	A	1114	CLA	CHA-CBD-CGD-O1D
15	A	1132	CLA	CHA-CBD-CGD-O1D
15	A	1132	CLA	CHA-CBD-CGD-O2D
15	4	612	CLA	CHA-CBD-CGD-O1D
15	4	612	CLA	CHA-CBD-CGD-O2D
15	2	615	CLA	CHA-CBD-CGD-O1D
15	B	1210	CLA	CHA-CBD-CGD-O1D
15	B	1210	CLA	CHA-CBD-CGD-O2D
15	2	603	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	CHA-CBD-CGD-O1D
15	A	1131	CLA	CHA-CBD-CGD-O2D
15	A	1125	CLA	CHA-CBD-CGD-O2D
16	1	610	CHL	C4C-C3C-CAC-CBC
15	2	601	CLA	O1A-CGA-O2A-C1
15	2	607	CLA	O1A-CGA-O2A-C1
15	A	1012	CLA	O1A-CGA-O2A-C1
15	B	1023	CLA	O1A-CGA-O2A-C1
21	4	811	DGD	O1G-C1G-C2G-O2G
21	2	811	DGD	O1G-C1G-C2G-O2G
15	A	1138	CLA	C4-C3-C5-C6
15	B	1203	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	C14-C13-C15-C16
15	1	615	CLA	C11-C12-C13-C14
19	1	811	SQD	C4-C5-C6-S
15	4	601	CLA	C2A-CAA-CBA-CGA
15	4	615	CLA	C2A-CAA-CBA-CGA
15	3	615	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	CAA-CBA-CGA-O2A
13	3	502	XAT	C31-C32-C33-C40
14	1	505	BCR	C36-C18-C19-C20
13	3	502	XAT	C31-C32-C33-C34
13	2	502	XAT	C7-C8-C9-C10
14	3	504	BCR	C7-C8-C9-C10
15	B	1229	CLA	C1A-C2A-CAA-CBA
15	B	1206	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	1	607	CLA	C1A-C2A-CAA-CBA
15	2	601	CLA	C2-C1-O2A-CGA
15	4	615	CLA	C2-C1-O2A-CGA
14	1	503	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	4	505	BCR	C15-C16-C17-C18
13	1	502	XAT	C29-C30-C31-C32
15	B	1239	CLA	C8-C10-C11-C12
17	2	801	LHG	C4-O6-P-O3
17	B	5001	LHG	C2-C3-O3-P
17	A	5001	LHG	C2-C3-O3-P
15	1	601	CLA	O2A-C1-C2-C3
16	2	609	CHL	O2A-C1-C2-C3
17	A	5001	LHG	O6-C4-C5-C6
15	A	1122	CLA	CAD-CBD-CGD-O1D
23	4	831	GSH	N1-CA1-CB1-CG1
15	A	1110	CLA	CAD-CBD-CGD-O1D
15	2	605	CLA	CAD-CBD-CGD-O1D
15	B	1210	CLA	CAD-CBD-CGD-O1D
15	A	1112	CLA	CAD-CBD-CGD-O1D
15	A	1135	CLA	CAD-CBD-CGD-O1D
15	A	1131	CLA	CAD-CBD-CGD-O1D
16	1	609	CHL	CAD-CBD-CGD-O1D
15	1	605	CLA	CAD-CBD-CGD-O1D
15	3	615	CLA	CAA-CBA-CGA-O2A
15	A	1103	CLA	C5-C6-C7-C8
15	A	1113	CLA	C2A-CAA-CBA-CGA
15	A	1013	CLA	C11-C12-C13-C15
15	A	1138	CLA	C11-C12-C13-C15
15	B	1231	CLA	C11-C10-C8-C7
12	1	501	LUT	C25-C26-C27-C28
15	A	1012	CLA	C11-C10-C8-C7
15	B	1021	CLA	C11-C10-C8-C7
15	1	615	CLA	C11-C12-C13-C15
12	3	501	LUT	C25-C26-C27-C28
15	B	1212	CLA	C3A-C2A-CAA-CBA
14	J	4002	BCR	C15-C16-C17-C18
15	A	1013	CLA	C2C-C3C-CAC-CBC
15	A	1106	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O7-C5-C6-O8
15	B	1228	CLA	C3-C5-C6-C7
15	B	1224	CLA	CBA-CGA-O2A-C1
15	A	1138	CLA	C2-C3-C5-C6
15	A	1104	CLA	C11-C10-C8-C9
15	B	1240	CLA	C14-C13-C15-C16
15	1	615	CLA	C11-C10-C8-C9
15	B	1224	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	4	613	CHL	C2A-CAA-CBA-CGA
15	3	610	CLA	CAA-CBA-CGA-O2A
14	B	4001	BCR	C18-C19-C20-C21
14	J	4003	BCR	C18-C19-C20-C21
14	4	505	BCR	C18-C19-C20-C21
14	A	4004	BCR	C18-C19-C20-C21
14	A	4007	BCR	C18-C19-C20-C21
14	A	4003	BCR	C18-C19-C20-C21
12	2	501	LUT	C29-C30-C31-C32
14	J	4001	BCR	C37-C22-C23-C24
15	4	607	CLA	CAA-CBA-CGA-O2A
15	4	604	CLA	C1-C2-C3-C4
15	B	1218	CLA	C1-C2-C3-C4
15	A	1119	CLA	C1-C2-C3-C4
15	A	1127	CLA	C1-C2-C3-C4
15	A	1134	CLA	C1-C2-C3-C4
15	B	1205	CLA	C1-C2-C3-C4
15	A	1117	CLA	C1-C2-C3-C4
15	B	1213	CLA	C1-C2-C3-C4
15	1	601	CLA	C1-C2-C3-C4
15	B	1214	CLA	C1-C2-C3-C4
15	4	601	CLA	C1-C2-C3-C4
15	4	607	CLA	C1-C2-C3-C4
15	A	1136	CLA	C1-C2-C3-C4
15	2	602	CLA	C1-C2-C3-C4
16	4	613	CHL	C1-C2-C3-C4
15	B	1230	CLA	C1-C2-C3-C4
15	A	1128	CLA	C1-C2-C3-C4
15	J	1302	CLA	C1-C2-C3-C4
15	B	1215	CLA	C1-C2-C3-C4
15	4	605	CLA	C1-C2-C3-C4
15	B	1224	CLA	C1-C2-C3-C4
15	B	1202	CLA	C1-C2-C3-C4
15	2	612	CLA	C1-C2-C3-C4
15	B	1203	CLA	C1-C2-C3-C4
15	3	610	CLA	C1-C2-C3-C4
15	B	1236	CLA	C1-C2-C3-C4
15	B	1206	CLA	C1-C2-C3-C4
15	B	1226	CLA	C1-C2-C3-C4
15	B	1216	CLA	C1-C2-C3-C4
15	A	1132	CLA	C1-C2-C3-C4
16	2	609	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
15	4	602	CLA	C1-C2-C3-C4
15	1	611	CLA	C1-C2-C3-C4
15	B	1222	CLA	C1-C2-C3-C4
15	B	1210	CLA	C1-C2-C3-C4
15	B	1234	CLA	C1-C2-C3-C4
15	B	1219	CLA	C1-C2-C3-C4
15	A	1126	CLA	C1-C2-C3-C4
15	B	1225	CLA	C1-C2-C3-C4
15	A	1121	CLA	C1-C2-C3-C4
15	A	1135	CLA	C1-C2-C3-C4
16	2	610	CHL	C1-C2-C3-C4
15	A	1137	CLA	C1-C2-C3-C4
15	B	1232	CLA	C1-C2-C3-C4
15	A	1125	CLA	C1-C2-C3-C4
15	A	1105	CLA	C1-C2-C3-C4
16	1	609	CHL	C1-C2-C3-C4
15	B	1237	CLA	C1-C2-C3-C4
15	A	1119	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C2A-CAA-CBA-CGA
15	B	1237	CLA	C2A-CAA-CBA-CGA
15	B	1218	CLA	C2-C1-O2A-CGA
24	A	1011	CL0	C2-C1-O2A-CGA
15	1	605	CLA	C2-C1-O2A-CGA
16	4	611	CHL	C2-C1-O2A-CGA
14	B	4001	BCR	C23-C24-C25-C26
14	F	4002	BCR	C5-C6-C7-C8
21	2	811	DGD	O1B-C1B-O2G-C2G
15	4	605	CLA	CAA-CBA-CGA-O2A
16	2	609	CHL	C4C-C3C-CAC-CBC
15	1	615	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	C4C-C3C-CAC-CBC
17	1	801	LHG	C4-O6-P-O3
17	2	801	LHG	C3-O3-P-O6
17	A	5001	LHG	C3-O3-P-O6
17	A	5002	LHG	C3-O3-P-O6
17	A	5002	LHG	C4-O6-P-O3
15	A	1012	CLA	C6-C7-C8-C9
13	3	502	XAT	C13-C14-C15-C35
14	2	503	BCR	C13-C14-C15-C16
12	3	501	LUT	C29-C30-C31-C32
14	A	4002	BCR	C13-C14-C15-C16
15	A	1137	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	1	612	CLA	C12-C13-C15-C16
18	1	802	LMG	O7-C10-C11-C12
15	B	1239	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C10-C11-C12-C13
15	2	602	CLA	CBA-CGA-O2A-C1
14	1	505	BCR	C17-C18-C19-C20
15	J	1302	CLA	O2A-C1-C2-C3
16	1	609	CHL	O2A-C1-C2-C3
15	B	1237	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C7-C8-C9-C10
15	A	1137	CLA	O1A-CGA-O2A-C1
15	B	1220	CLA	CAA-CBA-CGA-O1A
14	B	4003	BCR	C15-C16-C17-C18
15	B	1237	CLA	O1A-CGA-O2A-C1
13	4	502	XAT	C30-C31-C32-C33
16	2	610	CHL	CAA-CBA-CGA-O2A
15	B	1224	CLA	CAA-CBA-CGA-O2A
24	A	1011	CL0	CAA-CBA-CGA-O2A
16	2	610	CHL	C2-C1-O2A-CGA
15	B	1240	CLA	C8-C10-C11-C12
21	B	5002	DGD	O1A-C1A-C2A-C3A
15	2	607	CLA	C2A-CAA-CBA-CGA
15	4	605	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	3	611	CLA	C3A-C2A-CAA-CBA
14	J	4003	BCR	C13-C14-C15-C16
12	1	501	LUT	C29-C30-C31-C32
15	B	1231	CLA	C11-C10-C8-C9
14	4	505	BCR	C35-C13-C14-C15
14	4	505	BCR	C16-C17-C18-C36
14	1	505	BCR	C35-C13-C14-C15
12	1	501	LUT	C40-C33-C34-C35
14	F	4002	BCR	C16-C17-C18-C36
14	A	4004	BCR	C16-C17-C18-C36
14	A	4006	BCR	C16-C17-C18-C36
14	A	4007	BCR	C16-C17-C18-C36
15	B	1225	CLA	C2A-CAA-CBA-CGA
14	3	504	BCR	C17-C18-C19-C20
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	A	1132	CLA	C1A-C2A-CAA-CBA
15	A	1140	CLA	C1A-C2A-CAA-CBA
15	B	1210	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	B	1235	CLA	C6-C7-C8-C10
21	B	5002	DGD	O1G-C1A-C2A-C3A
17	A	5002	LHG	O8-C23-C24-C25
17	2	801	LHG	C2-C3-O3-P
15	B	1240	CLA	C2A-CAA-CBA-CGA
16	1	609	CHL	C2A-CAA-CBA-CGA
15	2	602	CLA	O1A-CGA-O2A-C1
15	B	1240	CLA	C15-C16-C17-C18
15	A	1138	CLA	C10-C11-C12-C13
14	4	505	BCR	C12-C13-C14-C15
14	4	505	BCR	C16-C17-C18-C19
14	1	505	BCR	C12-C13-C14-C15
12	1	501	LUT	C32-C33-C34-C35
14	F	4002	BCR	C16-C17-C18-C19
14	A	4004	BCR	C16-C17-C18-C19
14	A	4006	BCR	C16-C17-C18-C19
14	A	4007	BCR	C16-C17-C18-C19
14	4	505	BCR	C9-C10-C11-C12
14	A	4006	BCR	C9-C10-C11-C12
14	3	504	BCR	C15-C16-C17-C18
15	A	1138	CLA	C8-C10-C11-C12
15	3	601	CLA	C4C-C3C-CAC-CBC
15	B	1235	CLA	C2-C1-O2A-CGA
21	2	811	DGD	C2B-C1B-O2G-C2G
15	B	1240	CLA	CAA-CBA-CGA-O2A
15	A	1122	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	B	1219	CLA	C2A-CAA-CBA-CGA
16	2	610	CHL	C2C-C3C-CAC-CBC
14	B	4004	BCR	C1-C6-C7-C8
14	A	4005	BCR	C23-C24-C25-C30
14	A	4004	BCR	C1-C6-C7-C8
12	3	501	LUT	C1-C6-C7-C8
15	A	1103	CLA	C4-C3-C5-C6
21	B	5002	DGD	C5D-C6D-O5D-C1E
18	2	802	LMG	C8-C7-O1-C1
15	A	1121	CLA	CAA-CBA-CGA-O1A
16	4	610	CHL	C2A-CAA-CBA-CGA
15	B	1216	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	C4-C3-C5-C6
15	A	1103	CLA	C2-C3-C5-C6
14	J	4003	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	3	504	BCR	C13-C14-C15-C16
14	A	4003	BCR	C9-C10-C11-C12
17	1	801	LHG	C7-C8-C9-C10
17	A	5002	LHG	C2-C3-O3-P
16	2	610	CHL	O2A-C1-C2-C3
15	A	1138	CLA	CAA-CBA-CGA-O2A
15	B	1202	CLA	CAA-CBA-CGA-O2A
15	A	1105	CLA	CAA-CBA-CGA-O2A
25	B	2002	PQN	C25-C26-C27-C28
17	A	5002	LHG	O10-C23-C24-C25
15	A	1138	CLA	C11-C12-C13-C14
15	B	1240	CLA	C6-C7-C8-C9
15	B	1021	CLA	C11-C10-C8-C9
15	B	1235	CLA	C6-C7-C8-C9
15	B	1237	CLA	CAA-CBA-CGA-O1A
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	4	612	CLA	C3A-C2A-CAA-CBA
15	3	603	CLA	C3A-C2A-CAA-CBA
15	A	1119	CLA	CAA-CBA-CGA-O2A
15	B	1213	CLA	CAA-CBA-CGA-O2A
15	A	1134	CLA	CAD-CBD-CGD-O2D
15	B	1205	CLA	CAD-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O2D
16	2	609	CHL	CAD-CBD-CGD-O2D
15	1	608	CLA	CAD-CBD-CGD-O2D
16	2	613	CHL	CAD-CBD-CGD-O2D
14	B	4001	BCR	C15-C16-C17-C18
15	B	1217	CLA	C2A-CAA-CBA-CGA
15	4	609	CLA	CAA-CBA-CGA-O2A
15	B	1201	CLA	CAA-CBA-CGA-O2A
15	A	1013	CLA	C4C-C3C-CAC-CBC
15	B	1220	CLA	C4-C3-C5-C6
15	2	604	CLA	CAA-CBA-CGA-O1A
15	3	613	CLA	CAA-CBA-CGA-O2A
15	A	1132	CLA	CAA-CBA-CGA-O2A
15	3	601	CLA	CAA-CBA-CGA-O2A
15	4	603	CLA	CAA-CBA-CGA-O2A
14	J	4001	BCR	C21-C22-C23-C24
12	4	501	LUT	C31-C32-C33-C34
15	A	1133	CLA	CAA-CBA-CGA-O2A
15	4	601	CLA	CAA-CBA-CGA-O2A
15	2	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	A	1141	CLA	CAA-CBA-CGA-O2A
15	2	603	CLA	C2A-CAA-CBA-CGA
15	A	1137	CLA	CAA-CBA-CGA-O2A
15	A	1127	CLA	CHA-CBD-CGD-O1D
15	A	1127	CLA	CHA-CBD-CGD-O2D
15	A	1013	CLA	CHA-CBD-CGD-O2D
15	F	1301	CLA	CHA-CBD-CGD-O1D
15	F	1301	CLA	CHA-CBD-CGD-O2D
15	B	1213	CLA	CHA-CBD-CGD-O1D
15	B	1213	CLA	CHA-CBD-CGD-O2D
16	3	604	CHL	CHA-CBD-CGD-O1D
16	3	604	CHL	CHA-CBD-CGD-O2D
15	B	1214	CLA	CHA-CBD-CGD-O1D
15	B	1214	CLA	CHA-CBD-CGD-O2D
15	3	607	CLA	CHA-CBD-CGD-O1D
15	3	607	CLA	CHA-CBD-CGD-O2D
15	A	1136	CLA	CHA-CBD-CGD-O1D
15	A	1136	CLA	CHA-CBD-CGD-O2D
15	A	1113	CLA	CHA-CBD-CGD-O1D
15	A	1113	CLA	CHA-CBD-CGD-O2D
15	A	1122	CLA	CHA-CBD-CGD-O2D
15	2	604	CLA	CHA-CBD-CGD-O1D
15	2	604	CLA	CHA-CBD-CGD-O2D
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	4	615	CLA	CHA-CBD-CGD-O1D
15	4	615	CLA	CHA-CBD-CGD-O2D
15	4	605	CLA	CHA-CBD-CGD-O1D
15	4	605	CLA	CHA-CBD-CGD-O2D
15	2	612	CLA	CHA-CBD-CGD-O1D
15	2	612	CLA	CHA-CBD-CGD-O2D
15	B	1022	CLA	CHA-CBD-CGD-O1D
15	B	1022	CLA	CHA-CBD-CGD-O2D
15	B	1203	CLA	CHA-CBD-CGD-O1D
15	B	1203	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	CHA-CBD-CGD-O1D
15	B	1236	CLA	CHA-CBD-CGD-O2D
15	1	602	CLA	CHA-CBD-CGD-O1D
15	1	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1239	CLA	CHA-CBD-CGD-O1D
15	B	1239	CLA	CHA-CBD-CGD-O2D
15	A	1110	CLA	CHA-CBD-CGD-O1D
16	2	609	CHL	CHA-CBD-CGD-O2D
15	B	1217	CLA	CHA-CBD-CGD-O1D
15	B	1217	CLA	CHA-CBD-CGD-O2D
15	1	606	CLA	CHA-CBD-CGD-O1D
15	1	611	CLA	CHA-CBD-CGD-O1D
15	1	611	CLA	CHA-CBD-CGD-O2D
15	A	1120	CLA	CHA-CBD-CGD-O2D
15	B	1228	CLA	CHA-CBD-CGD-O1D
15	B	1228	CLA	CHA-CBD-CGD-O2D
15	B	1222	CLA	CHA-CBD-CGD-O1D
15	2	615	CLA	CHA-CBD-CGD-O2D
15	B	1023	CLA	CHA-CBD-CGD-O1D
15	B	1023	CLA	CHA-CBD-CGD-O2D
15	B	1221	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	CHA-CBD-CGD-O2D
15	A	1126	CLA	CHA-CBD-CGD-O1D
15	A	1126	CLA	CHA-CBD-CGD-O2D
15	A	1139	CLA	CHA-CBD-CGD-O2D
15	B	1201	CLA	CHA-CBD-CGD-O1D
15	B	1201	CLA	CHA-CBD-CGD-O2D
15	B	1225	CLA	CHA-CBD-CGD-O2D
16	2	610	CHL	CHA-CBD-CGD-O1D
16	2	610	CHL	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O1D
15	2	606	CLA	CHA-CBD-CGD-O1D
24	A	1011	CL0	CHA-CBD-CGD-O1D
24	A	1011	CL0	CHA-CBD-CGD-O2D
15	1	602	CLA	CAA-CBA-CGA-O2A
15	A	1140	CLA	CAA-CBA-CGA-O2A
15	1	611	CLA	CAA-CBA-CGA-O2A
15	A	1128	CLA	CAA-CBA-CGA-O2A
15	A	1118	CLA	CAA-CBA-CGA-O2A
15	B	1223	CLA	CAA-CBA-CGA-O2A
15	2	602	CLA	C2A-CAA-CBA-CGA
15	3	605	CLA	CBA-CGA-O2A-C1
15	B	1240	CLA	CBA-CGA-O2A-C1
15	1	607	CLA	CAA-CBA-CGA-O1A
15	A	1124	CLA	CAA-CBA-CGA-O2A
15	A	1127	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	1136	CLA	CAA-CBA-CGA-O2A
15	1	615	CLA	CAA-CBA-CGA-O2A
15	2	605	CLA	C11-C10-C8-C9
15	4	607	CLA	O2A-C1-C2-C3
15	1	611	CLA	O2A-C1-C2-C3
15	B	1219	CLA	O2A-C1-C2-C3
15	4	602	CLA	C2C-C3C-CAC-CBC
15	B	1231	CLA	C8-C10-C11-C12
16	4	613	CHL	CAA-CBA-CGA-O2A
15	B	1239	CLA	C16-C17-C18-C19
15	A	1109	CLA	C2A-CAA-CBA-CGA
15	1	604	CLA	C2A-CAA-CBA-CGA
21	2	811	DGD	O1A-C1A-C2A-C3A
15	A	1138	CLA	CAA-CBA-CGA-O1A
15	B	1202	CLA	CAA-CBA-CGA-O1A
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	A	1105	CLA	CAA-CBA-CGA-O1A
15	1	605	CLA	O2A-C1-C2-C3
16	2	611	CHL	C2-C1-O2A-CGA
15	A	1130	CLA	C1A-C2A-CAA-CBA
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	B	1022	CLA	C1A-C2A-CAA-CBA
15	3	611	CLA	C1A-C2A-CAA-CBA
15	1	605	CLA	C1A-C2A-CAA-CBA
23	4	831	GSH	OE1-CD1-CG1-CB1
15	A	1136	CLA	CAA-CBA-CGA-O1A
15	A	1133	CLA	CAA-CBA-CGA-O1A
15	4	601	CLA	CAA-CBA-CGA-O1A
15	B	1236	CLA	CAA-CBA-CGA-O1A
15	1	602	CLA	CAA-CBA-CGA-O1A
15	4	603	CLA	CAA-CBA-CGA-O1A
15	B	1201	CLA	CAA-CBA-CGA-O1A
15	1	601	CLA	C2A-CAA-CBA-CGA
15	3	606	CLA	C4C-C3C-CAC-CBC
15	1	615	CLA	C16-C17-C18-C20
15	3	613	CLA	CAA-CBA-CGA-O1A
15	A	1132	CLA	CAA-CBA-CGA-O1A
15	3	601	CLA	CAA-CBA-CGA-O1A
15	A	1140	CLA	CAA-CBA-CGA-O1A
15	A	1106	CLA	C13-C15-C16-C17
15	B	1213	CLA	CAA-CBA-CGA-O1A
15	2	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	1235	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	C3-O3-P-O5
15	A	1124	CLA	CAA-CBA-CGA-O1A
15	A	1119	CLA	CAA-CBA-CGA-O1A
15	A	1127	CLA	CAA-CBA-CGA-O1A
15	1	611	CLA	CAA-CBA-CGA-O1A
15	A	1117	CLA	O2A-C1-C2-C3
14	4	503	BCR	C23-C24-C25-C26
14	4	503	BCR	C23-C24-C25-C30
14	B	4002	BCR	C23-C24-C25-C30
14	A	4004	BCR	C5-C6-C7-C8
15	A	1141	CLA	CAA-CBA-CGA-O1A
15	1	615	CLA	CAA-CBA-CGA-O1A
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	2	612	CLA	C2C-C3C-CAC-CBC
15	B	1202	CLA	CAD-CBD-CGD-O1D
15	B	1216	CLA	CAD-CBD-CGD-O1D
15	A	1132	CLA	CAD-CBD-CGD-O1D
15	A	1120	CLA	CAD-CBD-CGD-O1D
15	A	1118	CLA	CAA-CBA-CGA-O1A
15	4	609	CLA	CAA-CBA-CGA-O1A
15	A	1137	CLA	CAA-CBA-CGA-O1A
15	B	1240	CLA	C11-C12-C13-C14
25	A	2001	PQN	C16-C17-C18-C19
15	B	1023	CLA	C6-C7-C8-C9
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	1	601	CLA	CAA-CBA-CGA-O2A
15	A	1109	CLA	CAA-CBA-CGA-O2A
15	2	607	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
15	4	612	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	CAA-CBA-CGA-O2A
16	3	604	CHL	CAA-CBA-CGA-O2A
15	B	1211	CLA	CAA-CBA-CGA-O2A
15	B	1234	CLA	CAA-CBA-CGA-O2A
15	2	603	CLA	CAA-CBA-CGA-O2A
15	A	1135	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	C5-C6-C7-C8
15	A	1108	CLA	C3A-C2A-CAA-CBA
25	B	2002	PQN	C22-C23-C25-C26
15	A	1104	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	2	605	CLA	C11-C10-C8-C7
15	1	605	CLA	C3A-C2A-CAA-CBA
15	A	1109	CLA	CAA-CBA-CGA-O1A
15	A	1128	CLA	CAA-CBA-CGA-O1A
15	B	1209	CLA	CAA-CBA-CGA-O2A
15	F	1302	CLA	CAA-CBA-CGA-O2A
15	B	1232	CLA	CAA-CBA-CGA-O2A
15	3	601	CLA	O2A-C1-C2-C3
15	A	1140	CLA	C3-C5-C6-C7
15	1	601	CLA	CAA-CBA-CGA-O1A
15	B	1209	CLA	CAA-CBA-CGA-O1A
15	4	612	CLA	CAA-CBA-CGA-O1A
15	B	1223	CLA	CAA-CBA-CGA-O1A
15	3	607	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	B	1211	CLA	CAA-CBA-CGA-O1A
15	2	607	CLA	CAA-CBA-CGA-O1A
15	B	1232	CLA	CAA-CBA-CGA-O1A
15	A	1125	CLA	CAA-CBA-CGA-O1A
15	4	606	CLA	CAA-CBA-CGA-O2A
15	B	1238	CLA	CAA-CBA-CGA-O2A
15	A	1012	CLA	C10-C11-C12-C13
15	1	615	CLA	C15-C16-C17-C18
15	3	607	CLA	CAA-CBA-CGA-O1A
15	A	1129	CLA	CAA-CBA-CGA-O1A
21	4	811	DGD	O1G-C1A-C2A-C3A
15	B	1216	CLA	CAA-CBA-CGA-O2A
15	B	1228	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

190 monomers are involved in 1272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	604	CLA	13	0
15	A	1124	CLA	14	0
15	A	1133	CLA	4	0
14	B	4001	BCR	2	0
15	2	608	CLA	5	0
13	3	502	XAT	23	0
15	2	601	CLA	15	0
15	B	1218	CLA	9	0
15	A	1119	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	4004	BCR	5	0
15	A	1127	CLA	8	0
15	A	1134	CLA	6	0
15	A	1130	CLA	4	0
12	4	501	LUT	18	0
14	4	503	BCR	8	0
15	B	1205	CLA	7	0
15	A	1117	CLA	7	0
15	A	1013	CLA	27	0
15	B	1213	CLA	4	0
15	4	603	CLA	6	0
15	3	612	CLA	9	0
19	1	811	SQD	4	0
15	1	601	CLA	12	0
15	B	1227	CLA	6	0
15	A	1108	CLA	9	0
15	B	1214	CLA	11	0
21	4	811	DGD	7	0
15	B	1229	CLA	7	0
15	3	607	CLA	1	0
25	B	2002	PQN	6	0
15	B	1202	CLA	6	0
21	B	5002	DGD	4	0
15	B	1209	CLA	2	0
16	4	610	CHL	5	0
15	4	607	CLA	5	0
15	B	1204	CLA	7	0
15	A	1136	CLA	9	0
15	B	1211	CLA	9	0
15	A	1106	CLA	14	0
15	A	1113	CLA	6	0
14	J	4003	BCR	4	0
15	4	608	CLA	4	0
15	F	1301	CLA	6	0
23	4	831	GSH	0	1
15	2	602	CLA	7	0
16	4	613	CHL	7	0
15	2	607	CLA	8	0
15	B	1230	CLA	15	0
14	1	503	BCR	8	0
15	3	613	CLA	15	0
15	1	604	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	J	4002	BCR	15	0
15	2	604	CLA	6	0
14	B	4006	BCR	10	0
15	A	1138	CLA	13	0
20	4	902	CAC	1	0
15	A	1128	CLA	12	0
15	J	1302	CLA	8	0
15	B	1231	CLA	11	0
14	4	505	BCR	4	0
13	4	502	XAT	5	0
15	A	1118	CLA	2	0
15	4	615	CLA	7	0
15	A	1129	CLA	2	0
18	2	802	LMG	1	0
15	B	1215	CLA	7	0
15	4	605	CLA	10	0
15	B	1224	CLA	5	0
15	A	1104	CLA	5	0
15	2	612	CLA	11	0
15	A	1115	CLA	6	0
15	3	605	CLA	12	0
15	A	1114	CLA	6	0
15	B	1022	CLA	10	0
15	3	615	CLA	2	0
15	4	601	CLA	13	0
15	B	1203	CLA	5	0
14	1	505	BCR	7	0
15	1	613	CLA	25	0
12	1	501	LUT	11	0
15	B	1220	CLA	5	0
15	3	610	CLA	5	0
15	B	1236	CLA	4	0
15	A	1111	CLA	23	0
17	B	5001	LHG	2	0
15	4	606	CLA	10	0
15	B	1206	CLA	5	0
15	1	602	CLA	2	0
15	B	1226	CLA	10	0
15	B	1239	CLA	11	0
15	B	1216	CLA	7	0
17	1	801	LHG	2	0
15	A	1012	CLA	30	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1110	CLA	16	0
14	2	503	BCR	8	0
15	A	1109	CLA	13	0
15	A	1132	CLA	5	0
16	2	609	CHL	15	0
15	B	1240	CLA	5	0
15	B	1217	CLA	2	0
21	2	811	DGD	2	0
15	A	1122	CLA	5	0
15	B	1221	CLA	8	0
15	1	606	CLA	15	0
15	B	1021	CLA	25	0
14	B	4002	BCR	3	0
15	4	612	CLA	12	0
15	1	611	CLA	9	0
20	3	902	CAC	1	0
15	B	1235	CLA	12	0
15	3	601	CLA	15	0
13	2	502	XAT	15	0
15	B	1223	CLA	6	0
15	A	1107	CLA	11	0
15	A	1120	CLA	1	0
15	A	1141	CLA	4	0
15	B	1228	CLA	9	0
18	1	802	LMG	1	0
15	4	602	CLA	8	0
16	1	610	CHL	16	0
15	2	605	CLA	7	0
15	B	1222	CLA	9	0
15	1	612	CLA	7	0
15	2	615	CLA	1	0
14	F	4002	BCR	6	0
15	A	1140	CLA	6	0
14	A	4005	BCR	14	0
15	A	1123	CLA	11	0
17	2	801	LHG	2	0
15	B	1023	CLA	19	0
15	B	1210	CLA	9	0
15	1	615	CLA	5	0
14	A	4004	BCR	4	0
15	4	609	CLA	11	0
15	A	1116	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	4003	BCR	8	0
14	J	4001	BCR	7	0
14	A	4006	BCR	8	0
14	3	504	BCR	5	0
15	B	1234	CLA	7	0
14	3	503	BCR	21	0
25	A	2001	PQN	12	0
16	2	611	CHL	5	0
17	A	5001	LHG	2	0
15	B	1219	CLA	8	0
14	A	4007	BCR	8	0
15	A	1126	CLA	9	0
15	2	603	CLA	3	0
15	A	1112	CLA	1	0
15	A	1139	CLA	11	0
26	C	3003	SF4	2	0
15	B	1201	CLA	4	0
15	1	603	CLA	13	0
15	B	1225	CLA	6	0
15	F	1302	CLA	6	0
15	A	1121	CLA	4	0
15	A	1135	CLA	5	0
15	A	1101	CLA	7	0
14	A	4003	BCR	2	0
15	1	608	CLA	14	0
16	2	610	CHL	5	0
15	3	608	CLA	5	0
16	3	604	CHL	14	0
15	A	1137	CLA	7	0
15	B	1238	CLA	1	0
17	A	5002	LHG	4	0
15	B	1232	CLA	8	0
15	3	603	CLA	22	0
12	2	501	LUT	12	0
23	B	5031	GSH	2	0
15	3	606	CLA	18	0
15	A	1131	CLA	3	0
15	A	1125	CLA	11	0
15	A	1105	CLA	7	0
16	1	609	CHL	11	0
14	B	4005	BCR	6	0
12	3	501	LUT	11	0

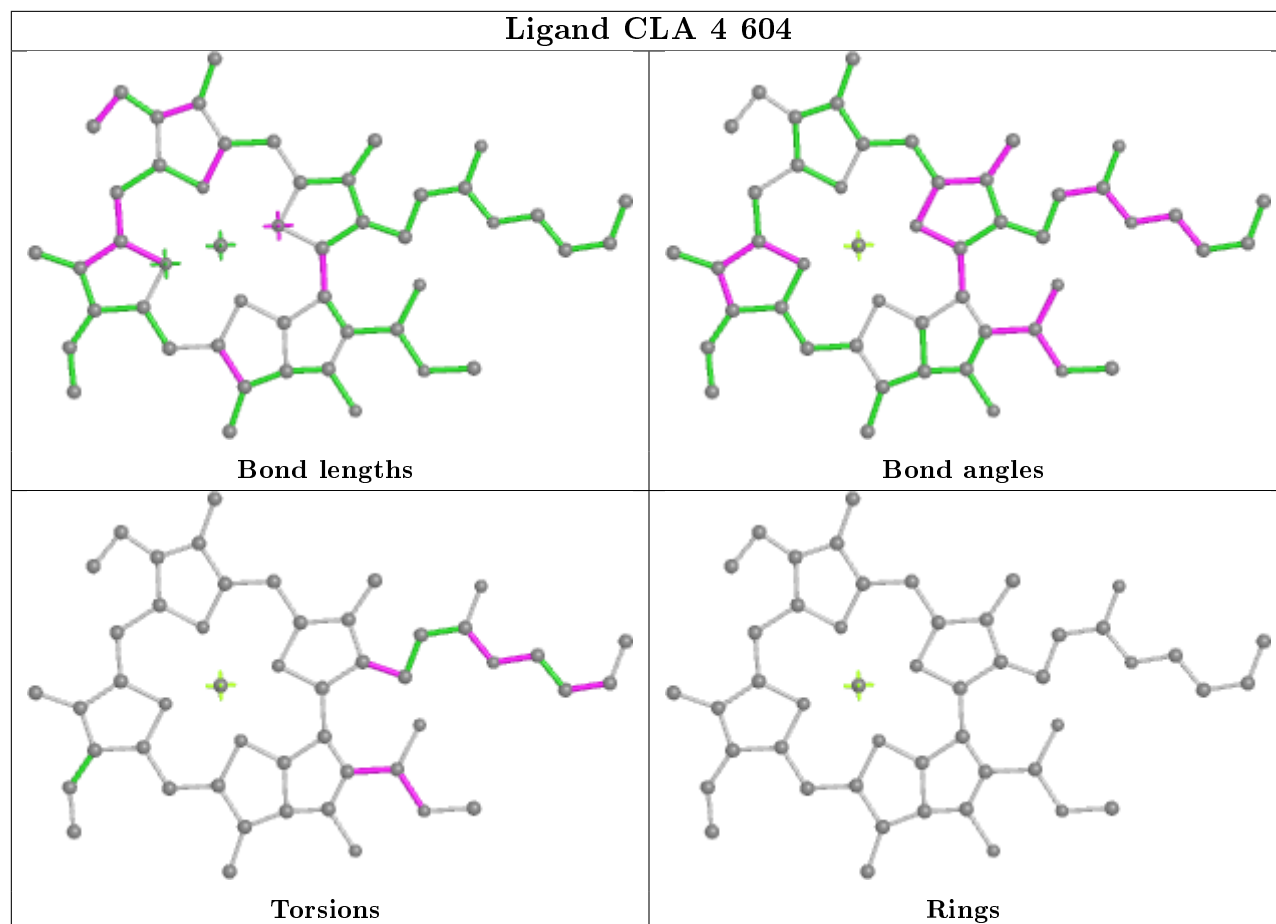
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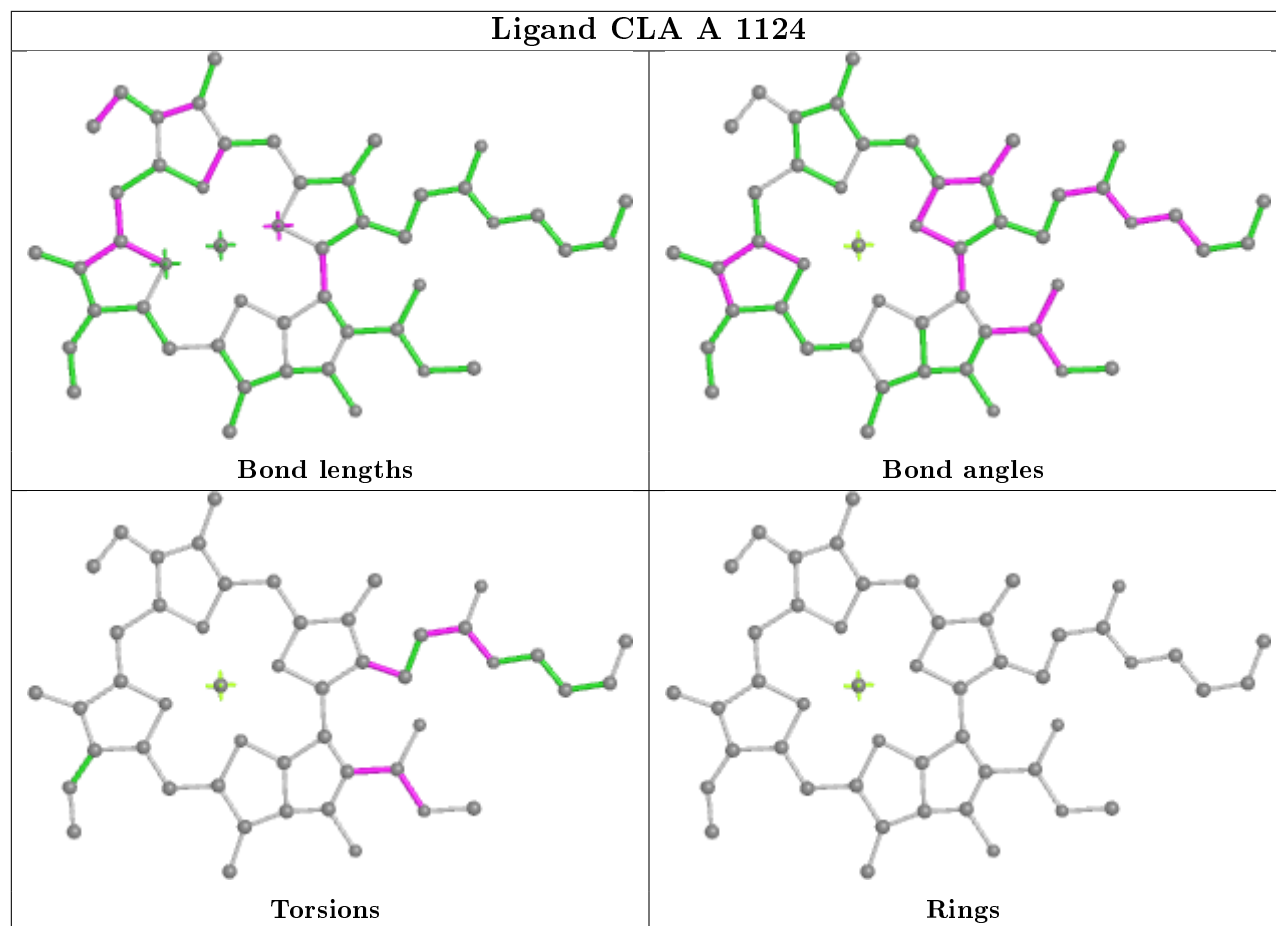
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1237	CLA	3	0
15	3	611	CLA	8	0
13	1	502	XAT	12	0
15	1	607	CLA	5	0
15	B	1212	CLA	7	0
16	2	613	CHL	6	0
15	2	606	CLA	7	0
15	A	1102	CLA	6	0
24	A	1011	CL0	23	0
15	A	1103	CLA	10	0
15	1	605	CLA	12	0
14	A	4002	BCR	6	0
16	4	611	CHL	9	0

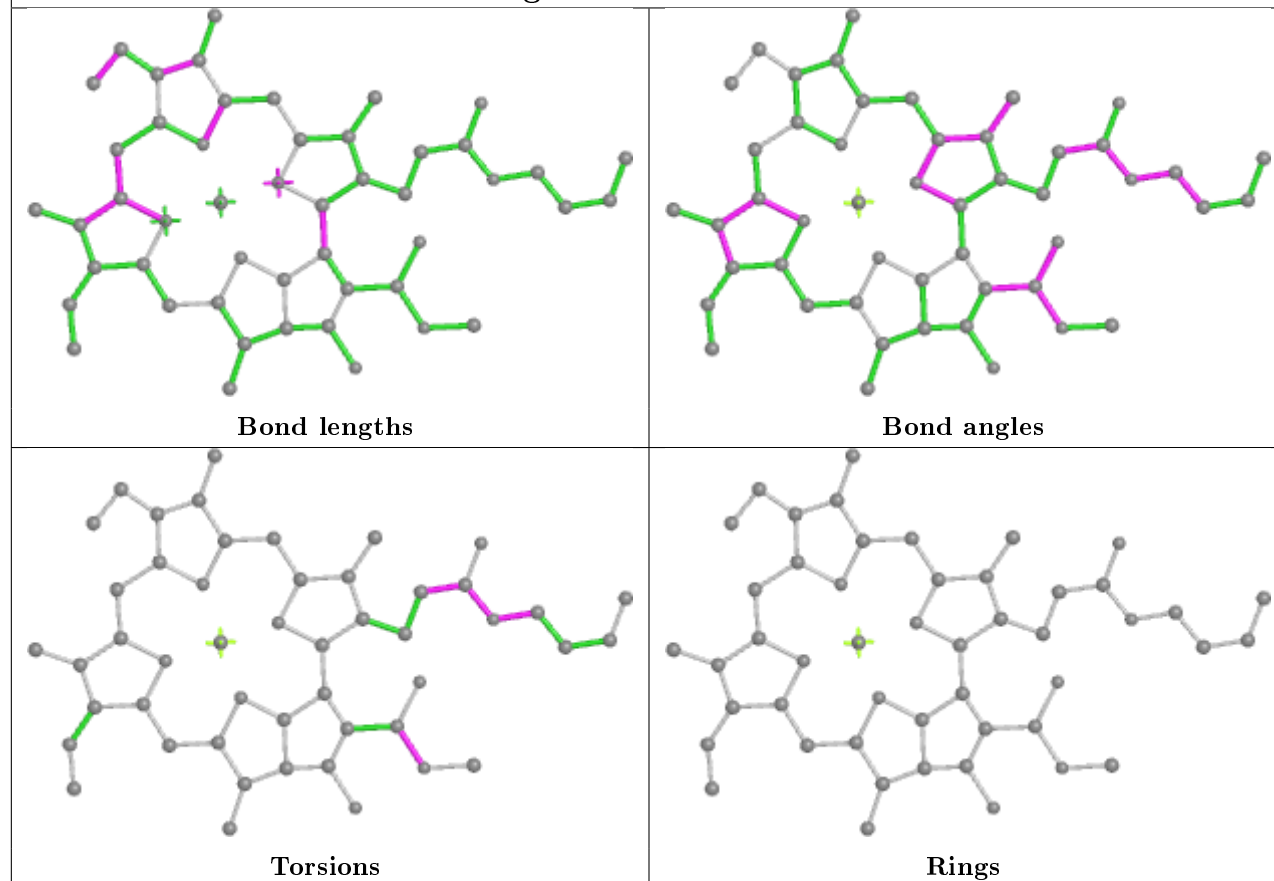
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA 4 604

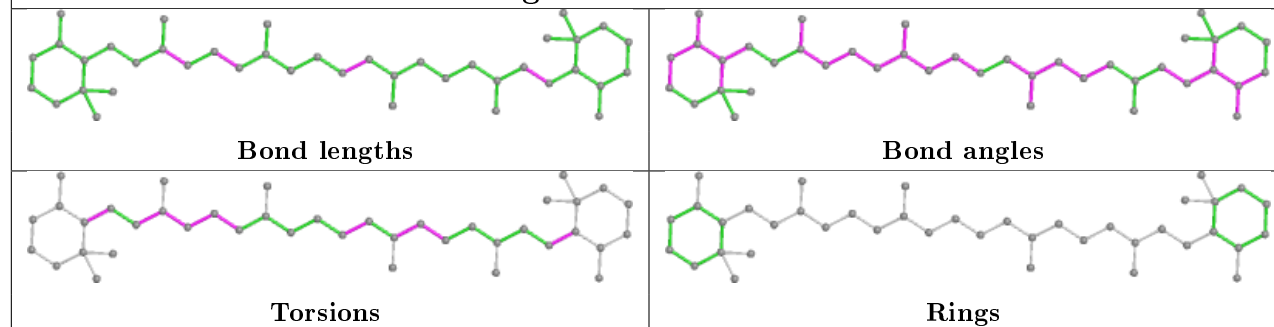




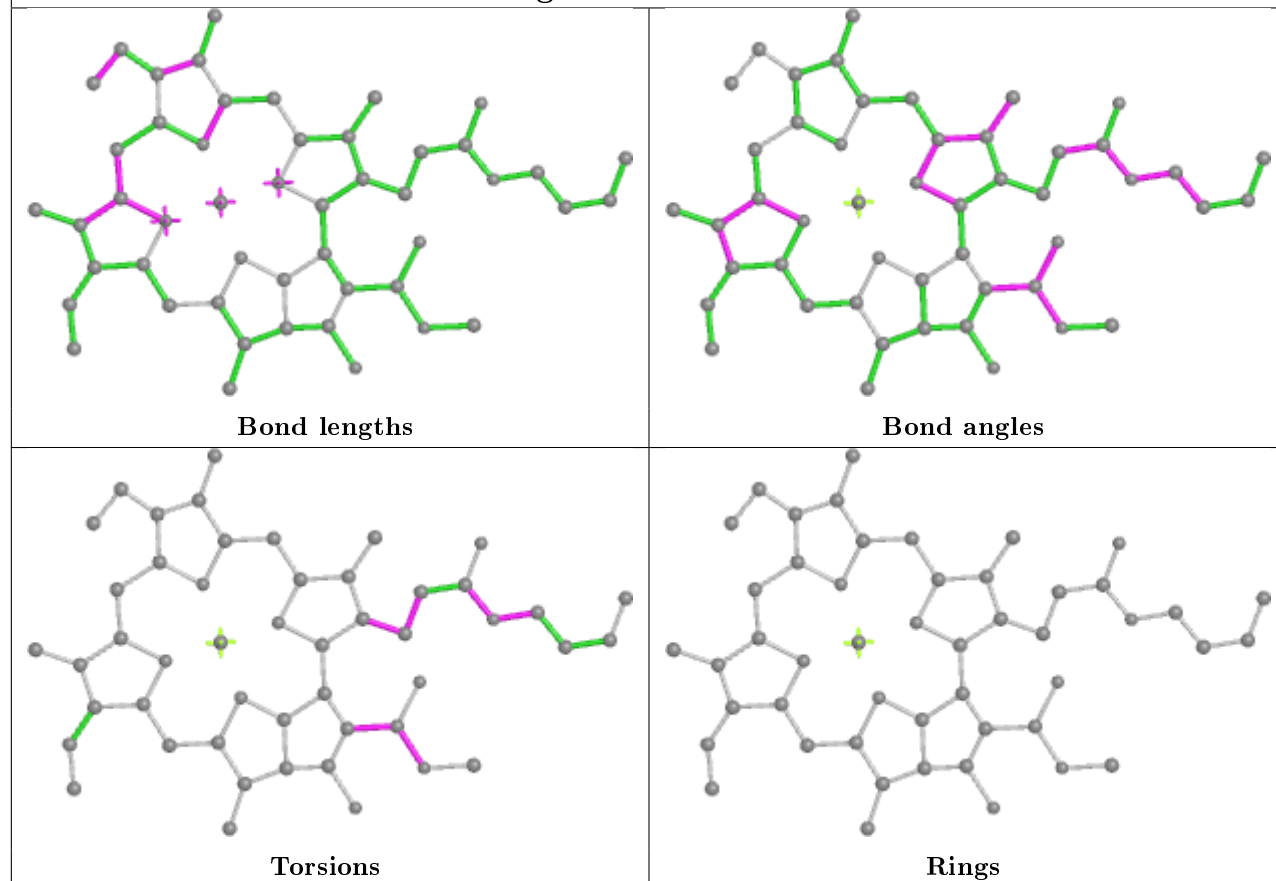
Ligand CLA A 1133



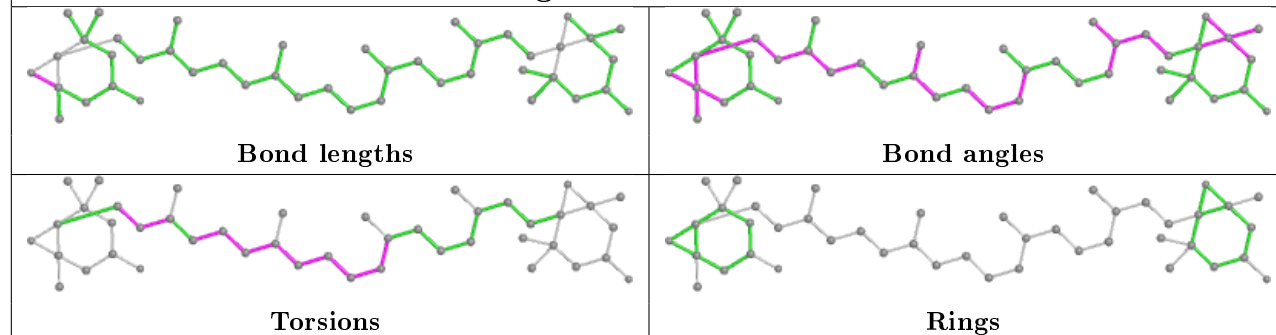
Ligand BCR B 4001



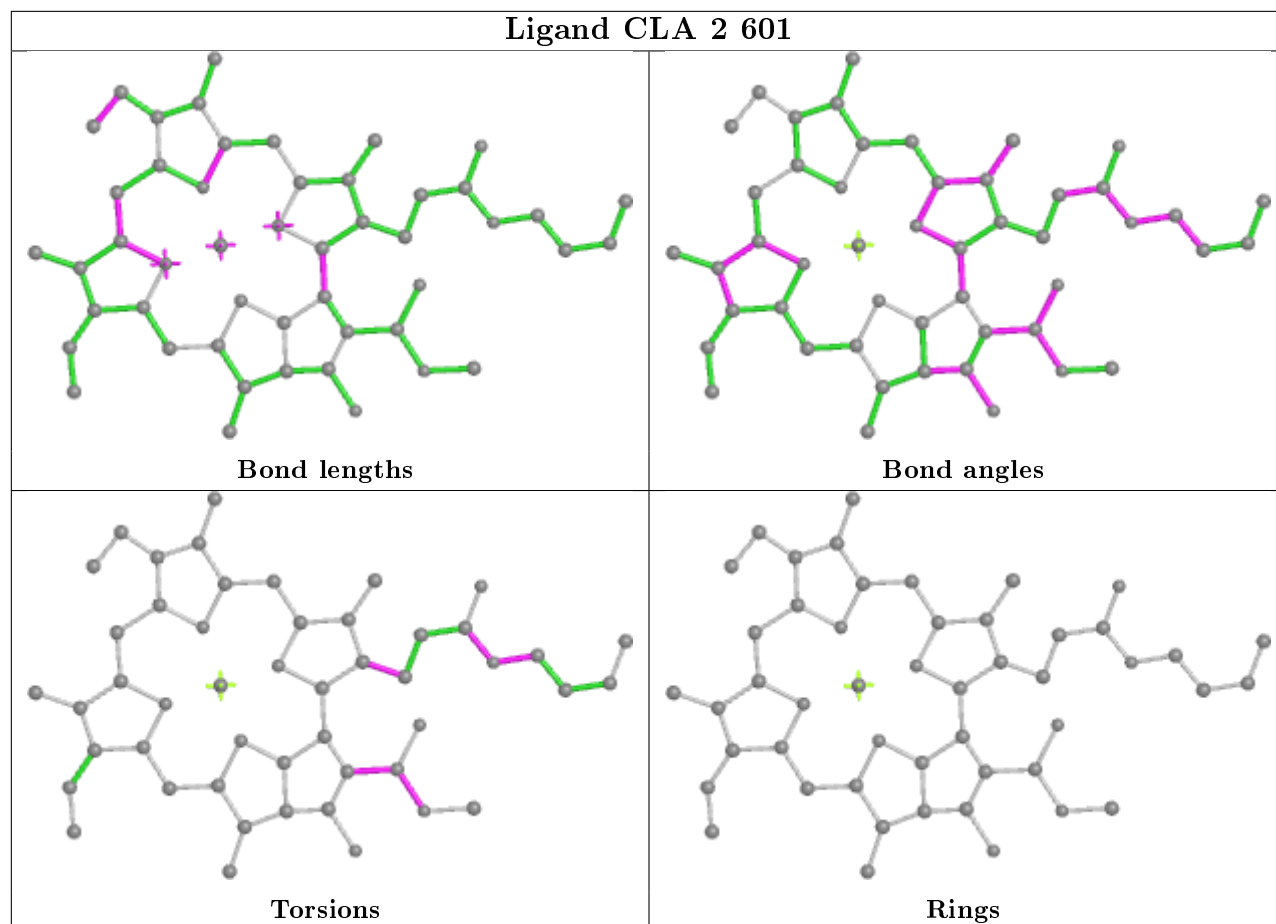
Ligand CLA 2 608

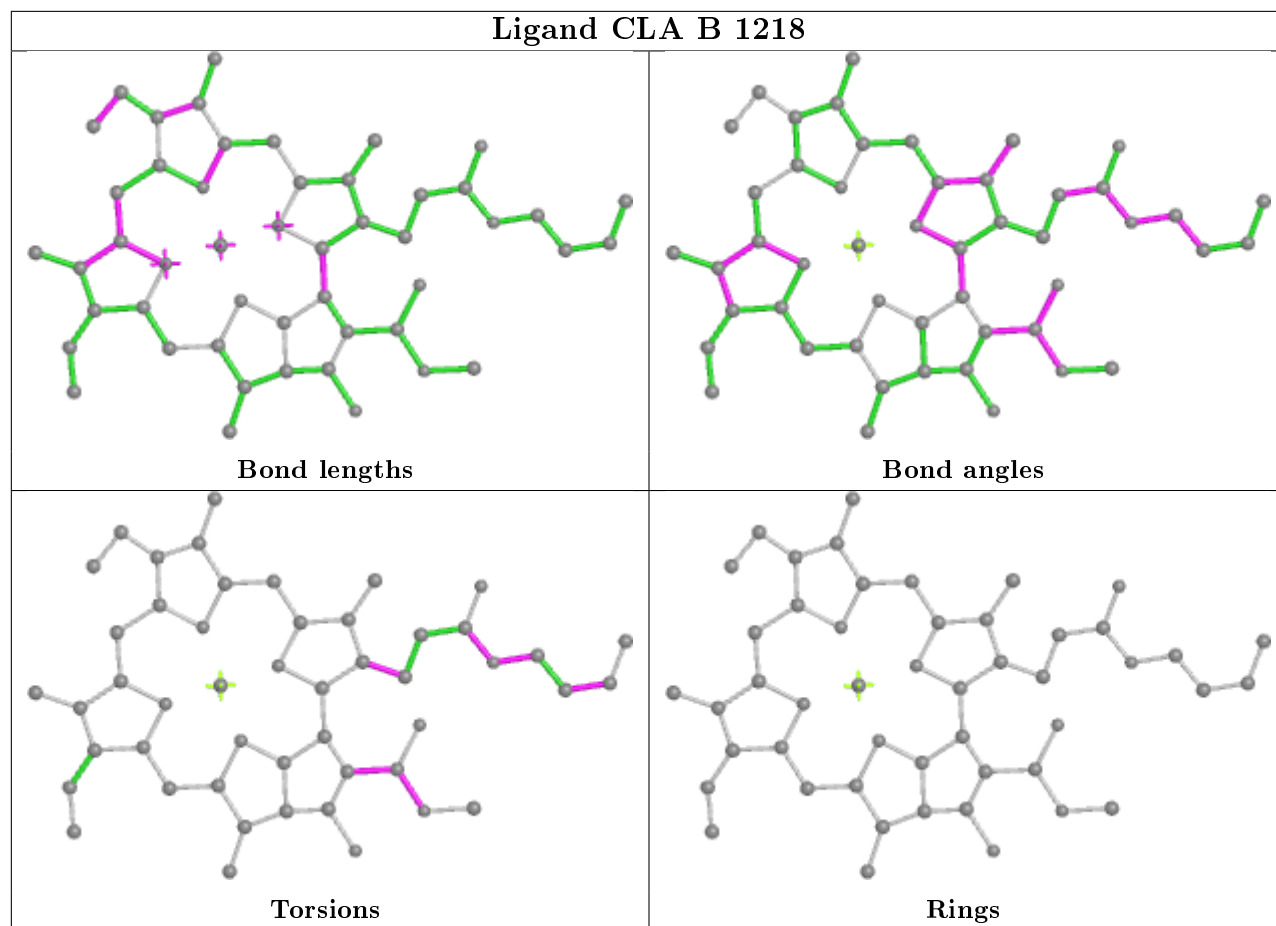


Ligand XAT 3 502

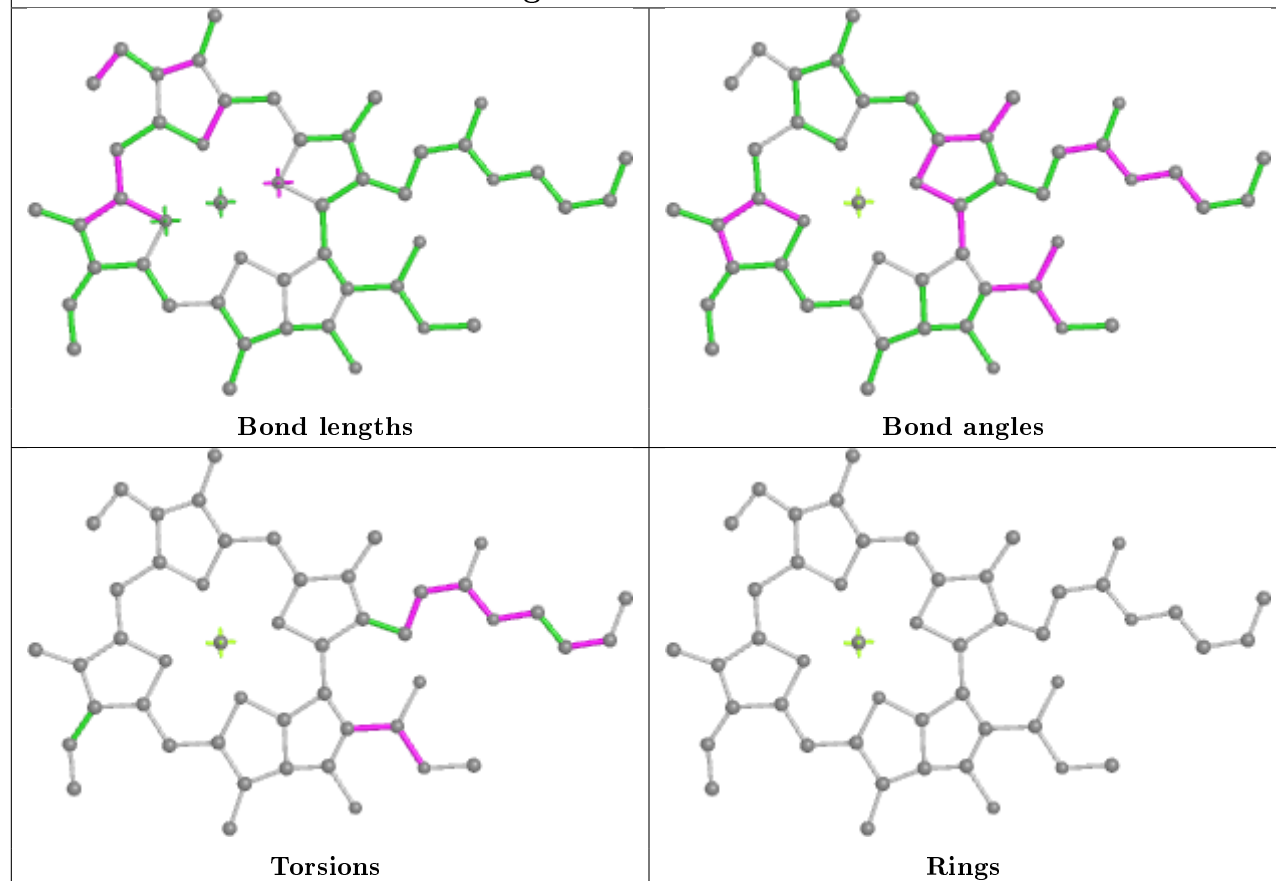


Ligand CLA 2 601

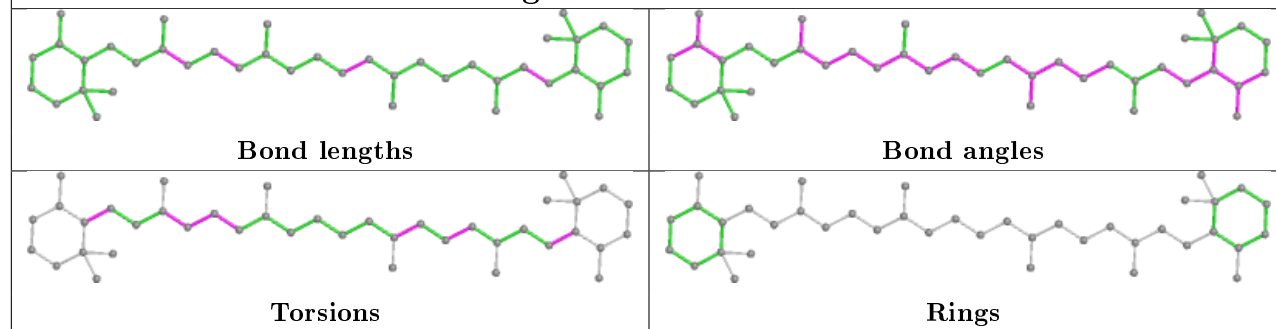


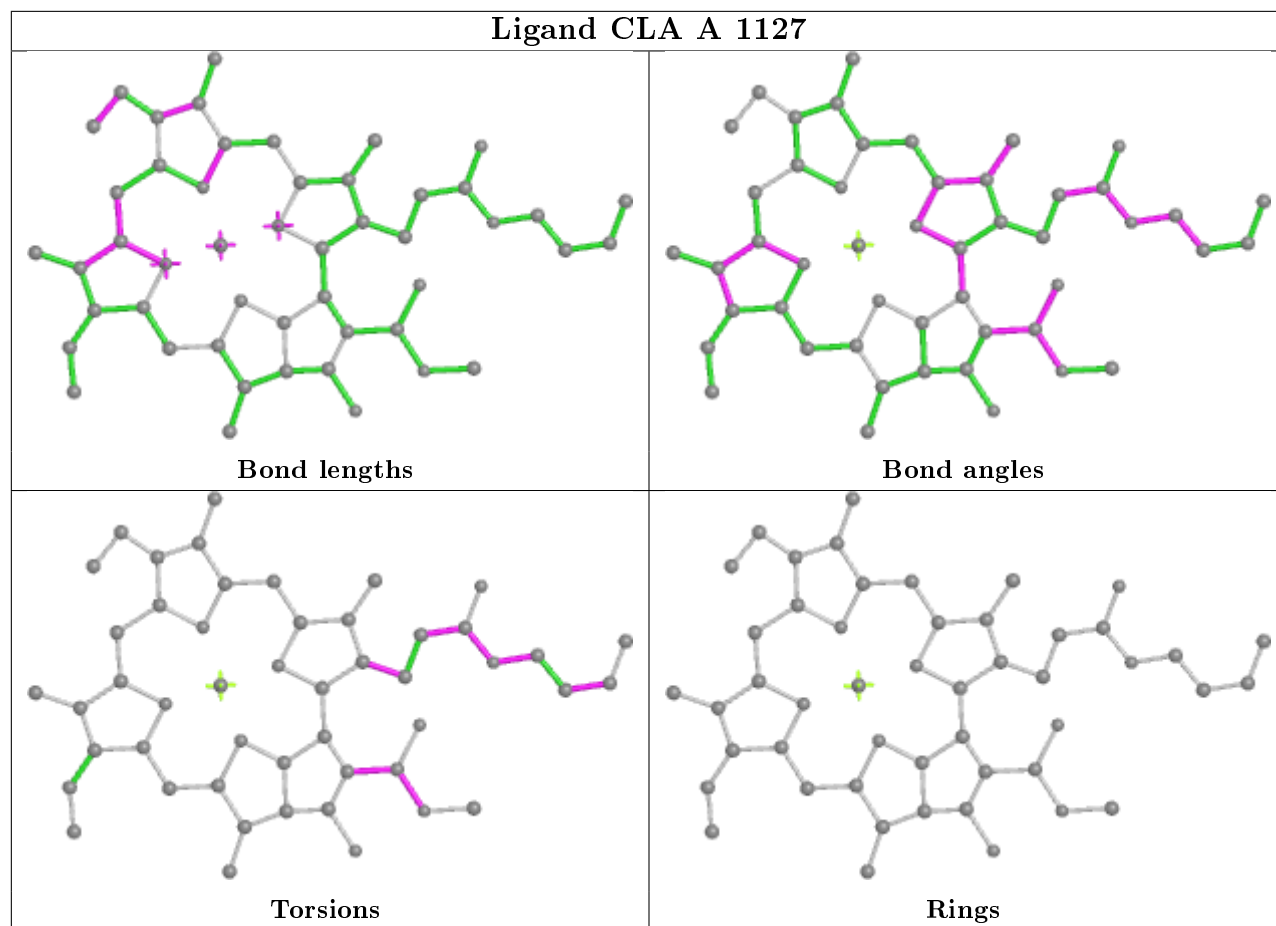


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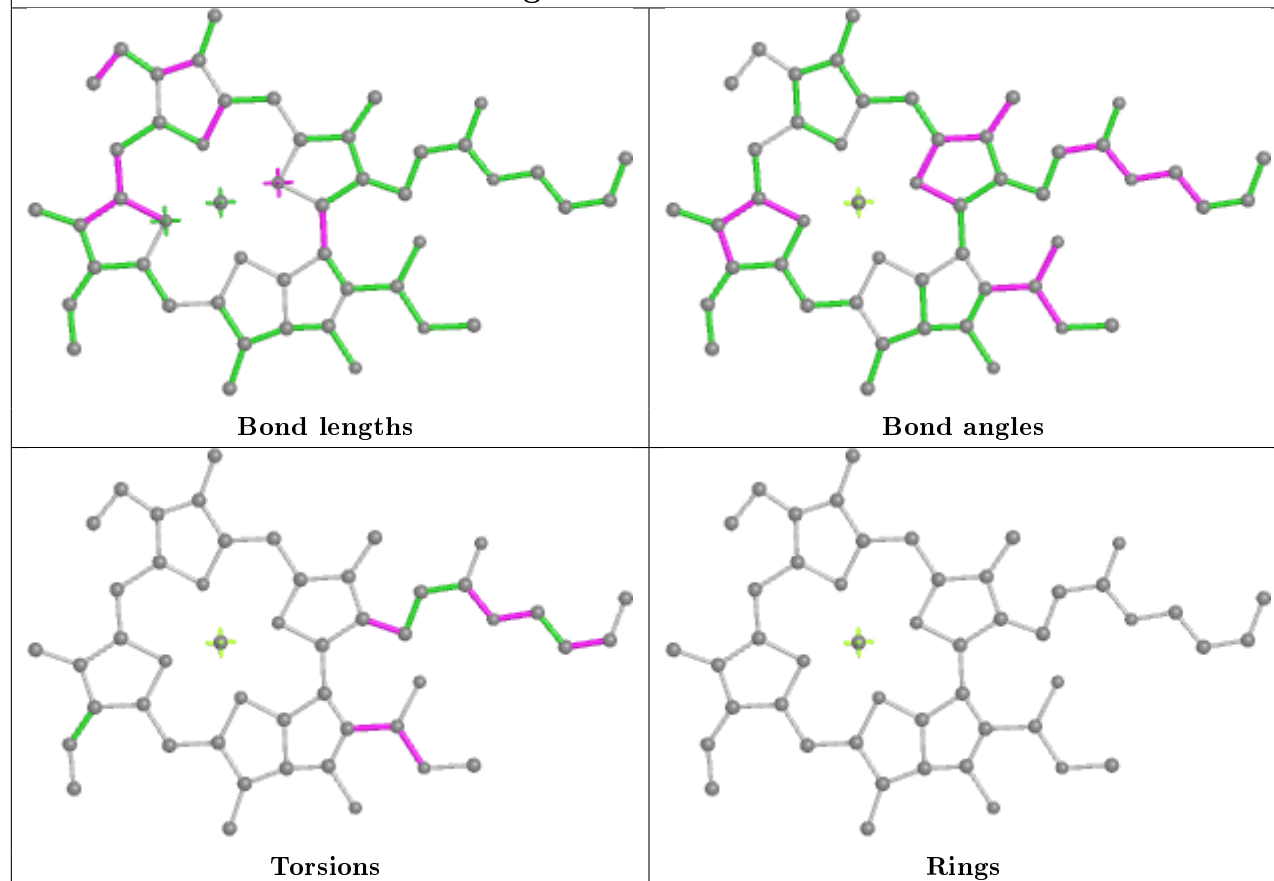


Ligand BCR B 4004

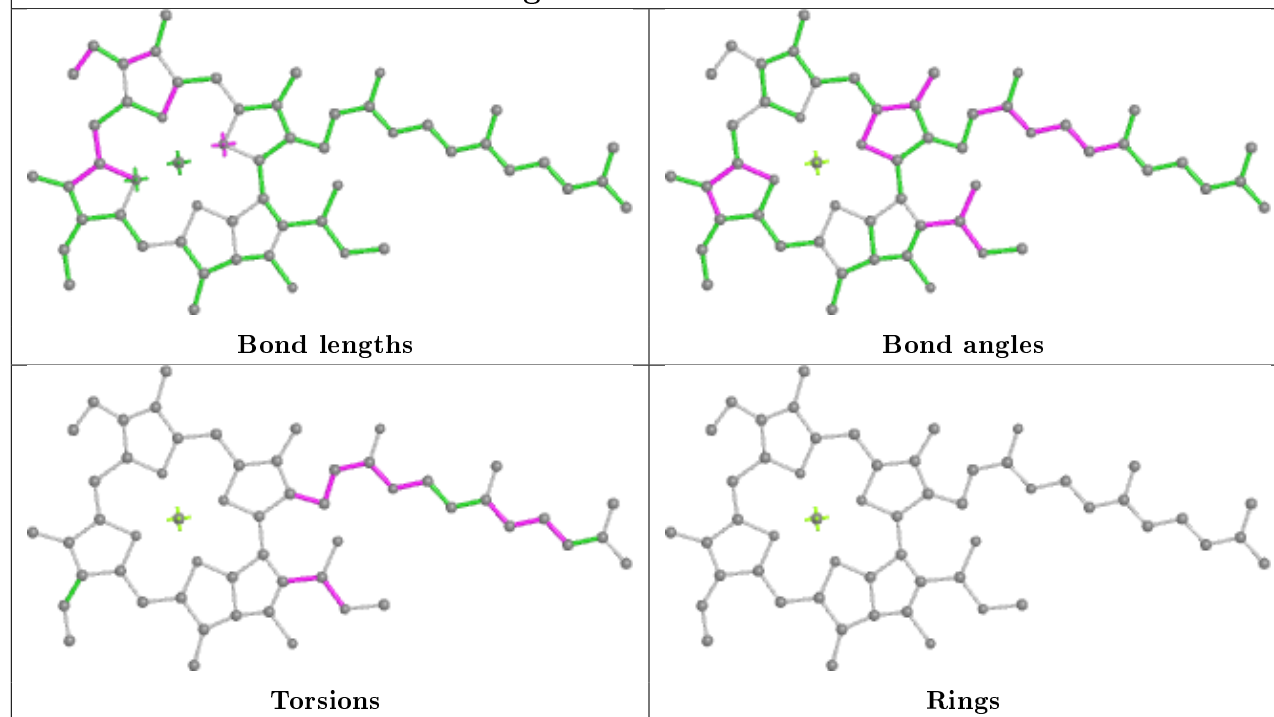


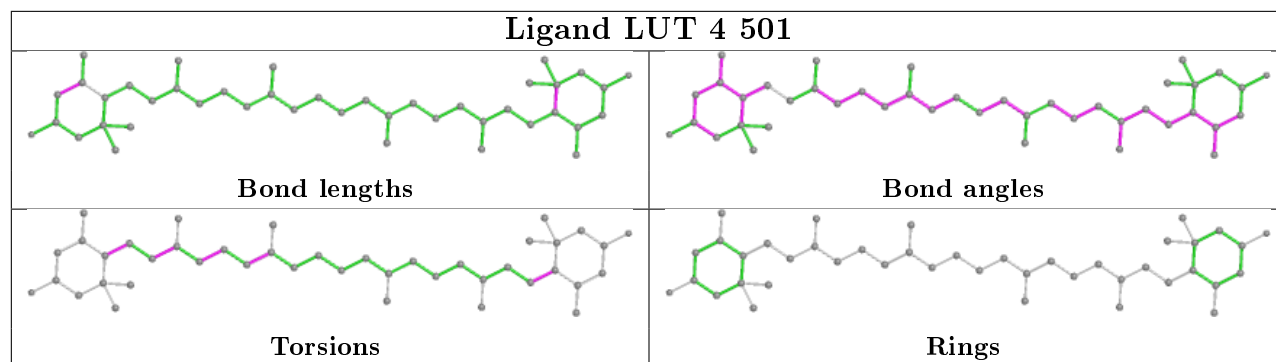
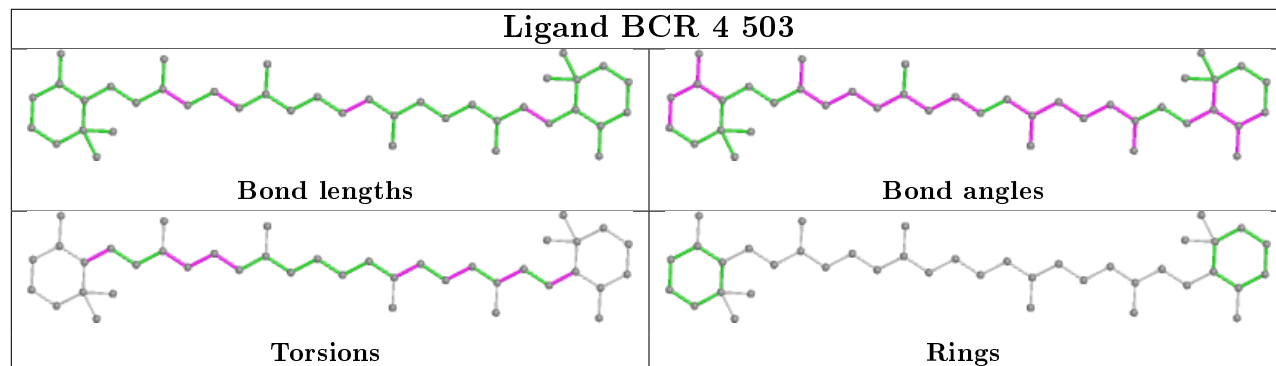
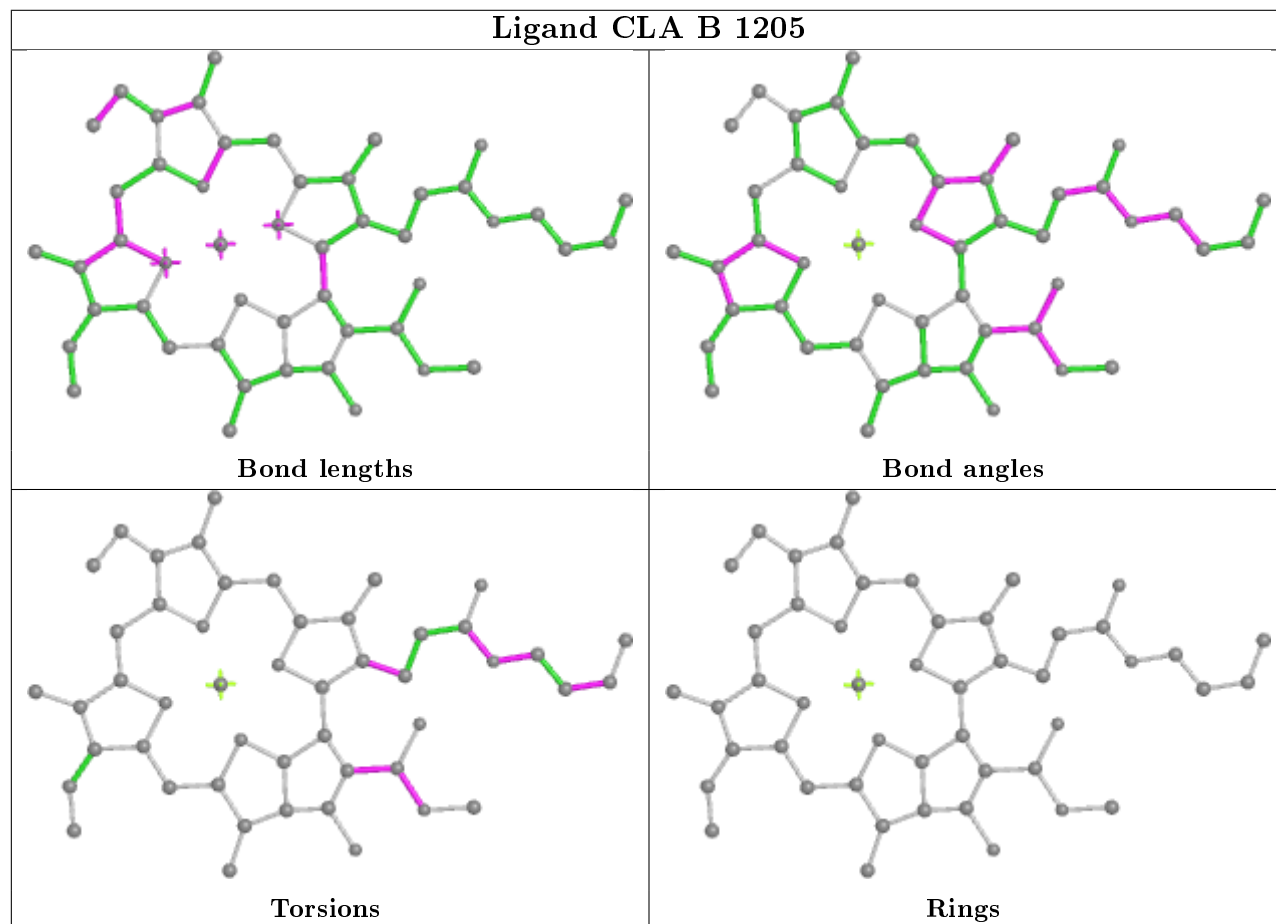


Ligand CLA A 1134

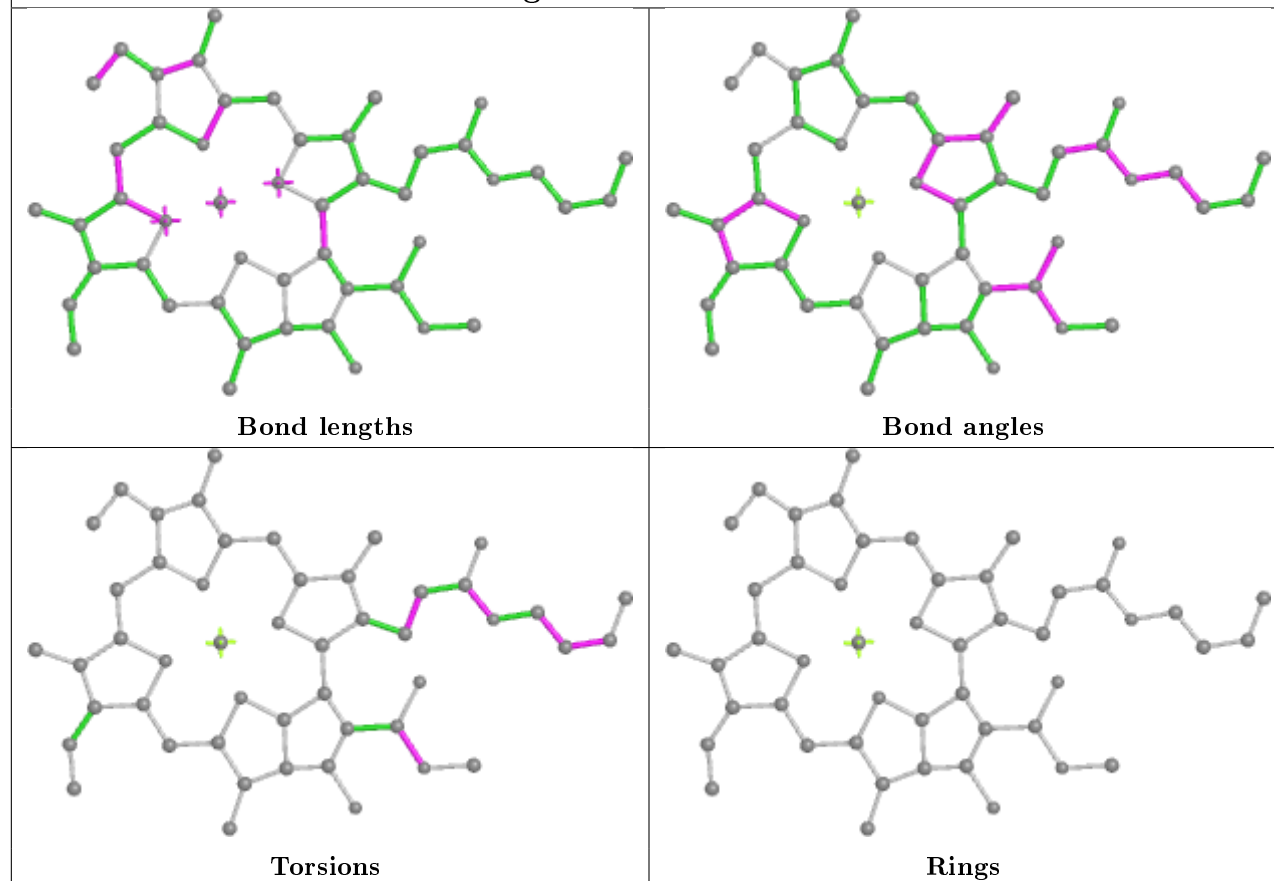


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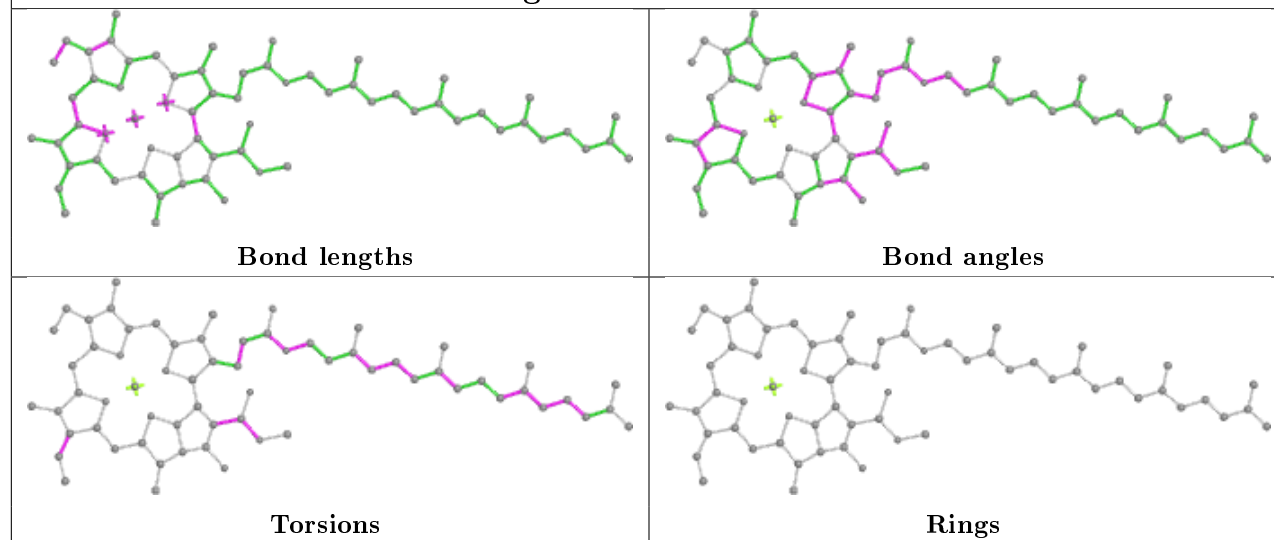


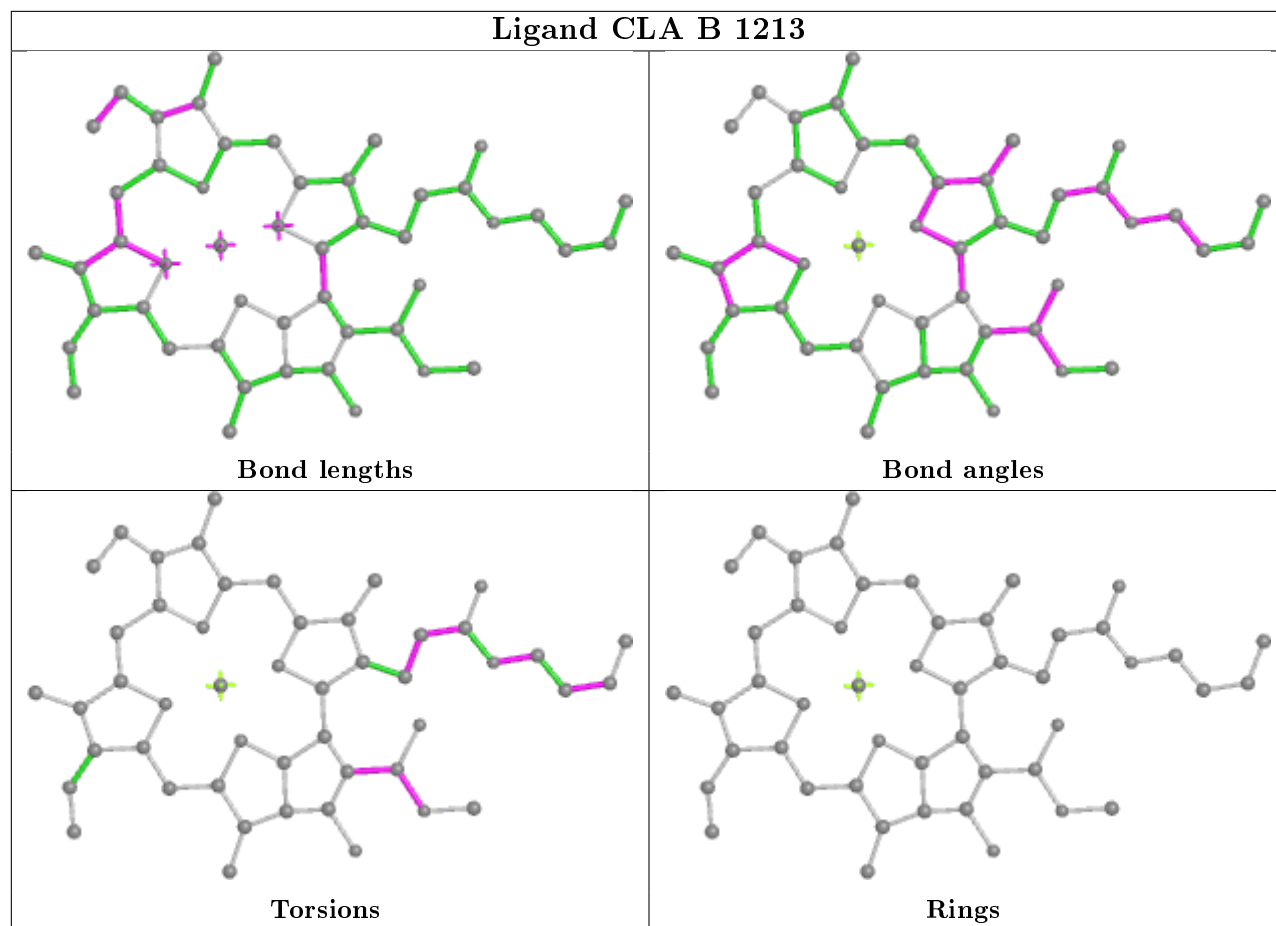
Ligand LUT 4 501**Ligand BCR 4 503****Ligand CLA B 1205**

Ligand CLA A 1117

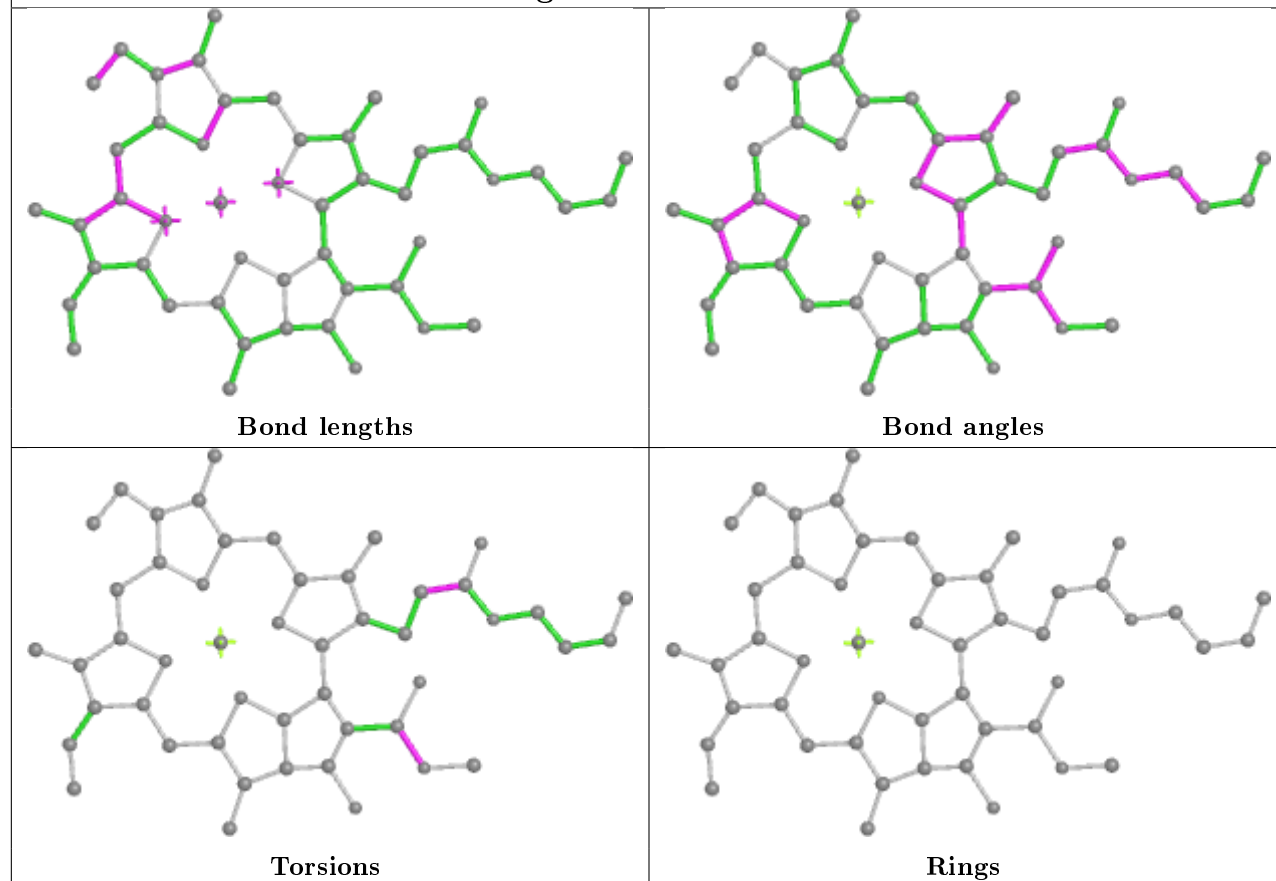


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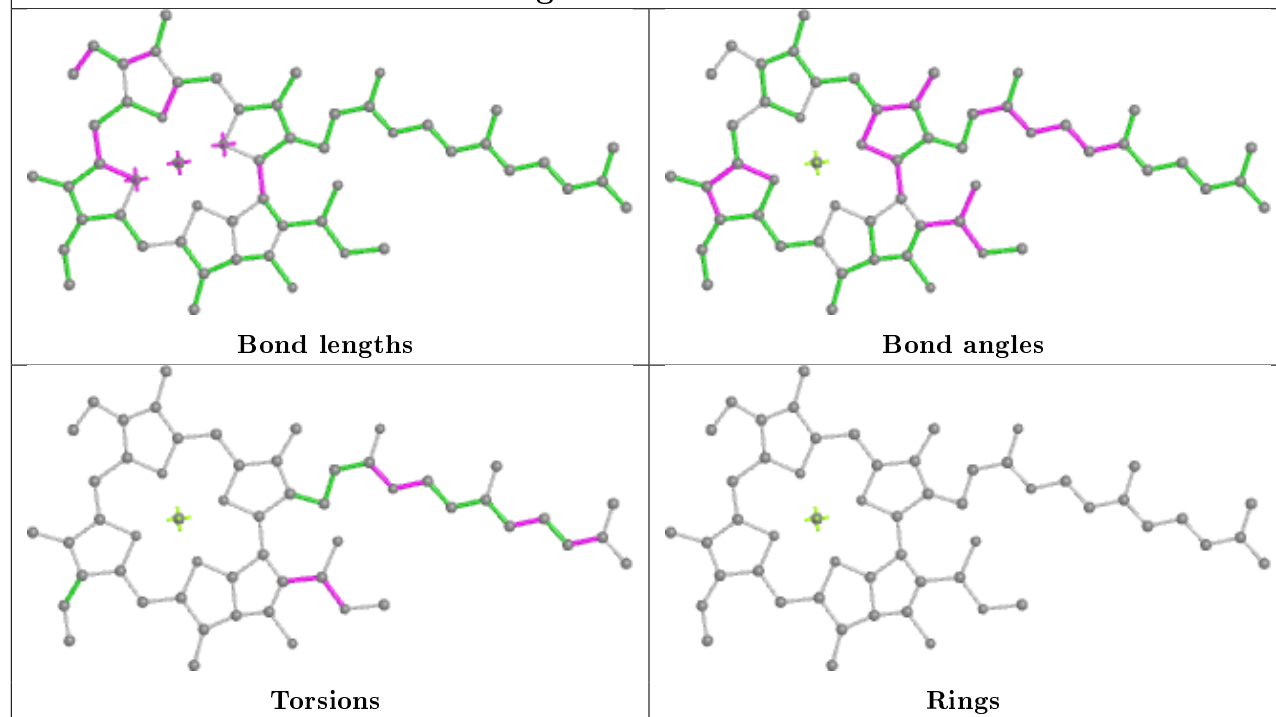




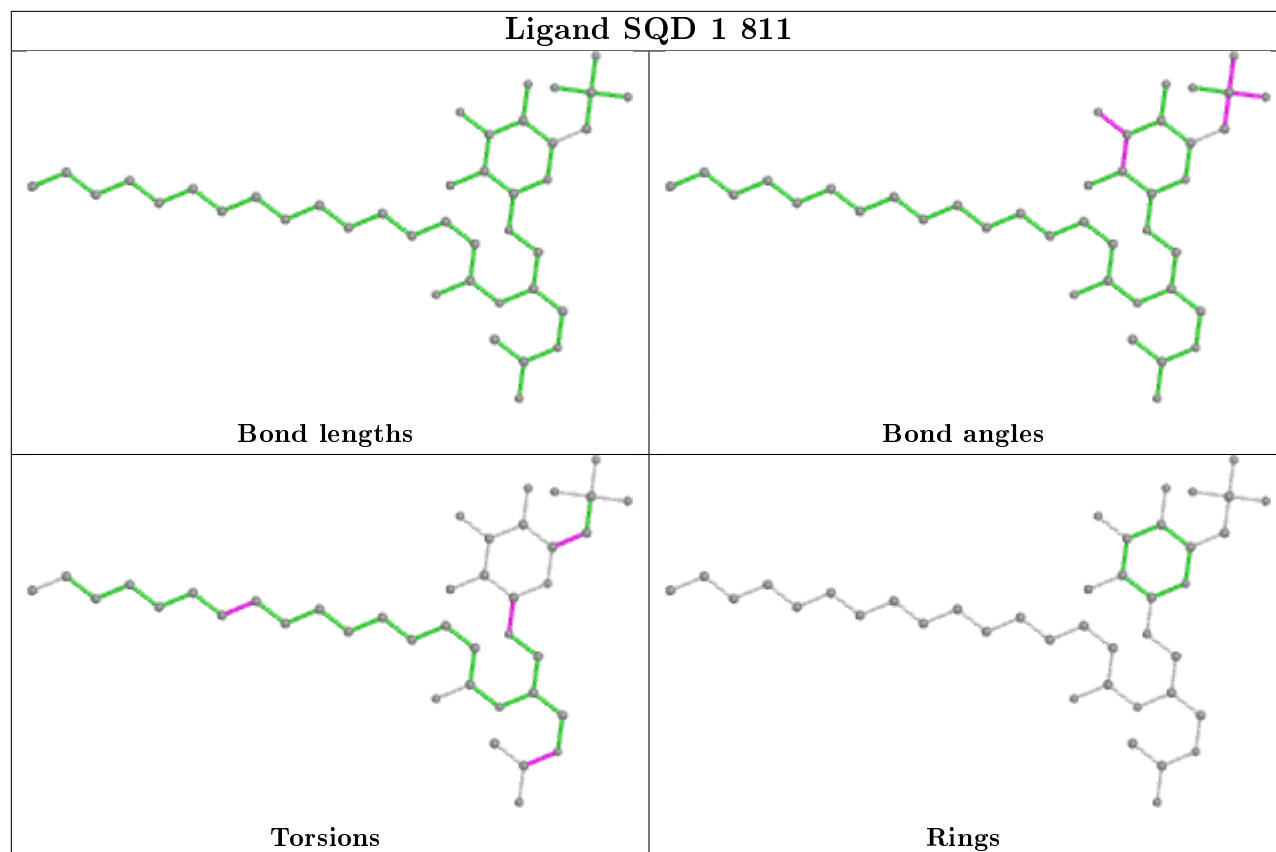
Ligand CLA 4 603



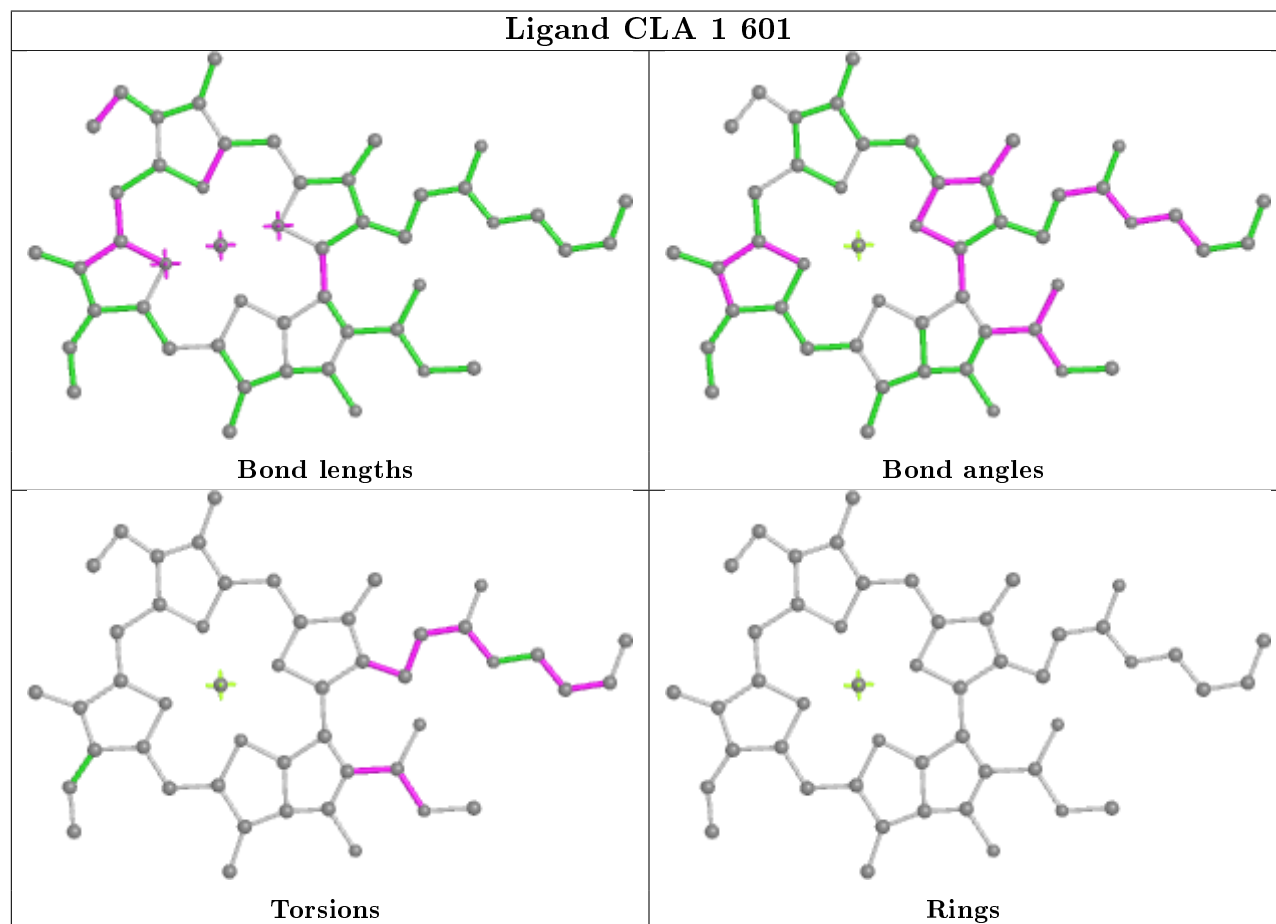
Ligand CLA 3 612



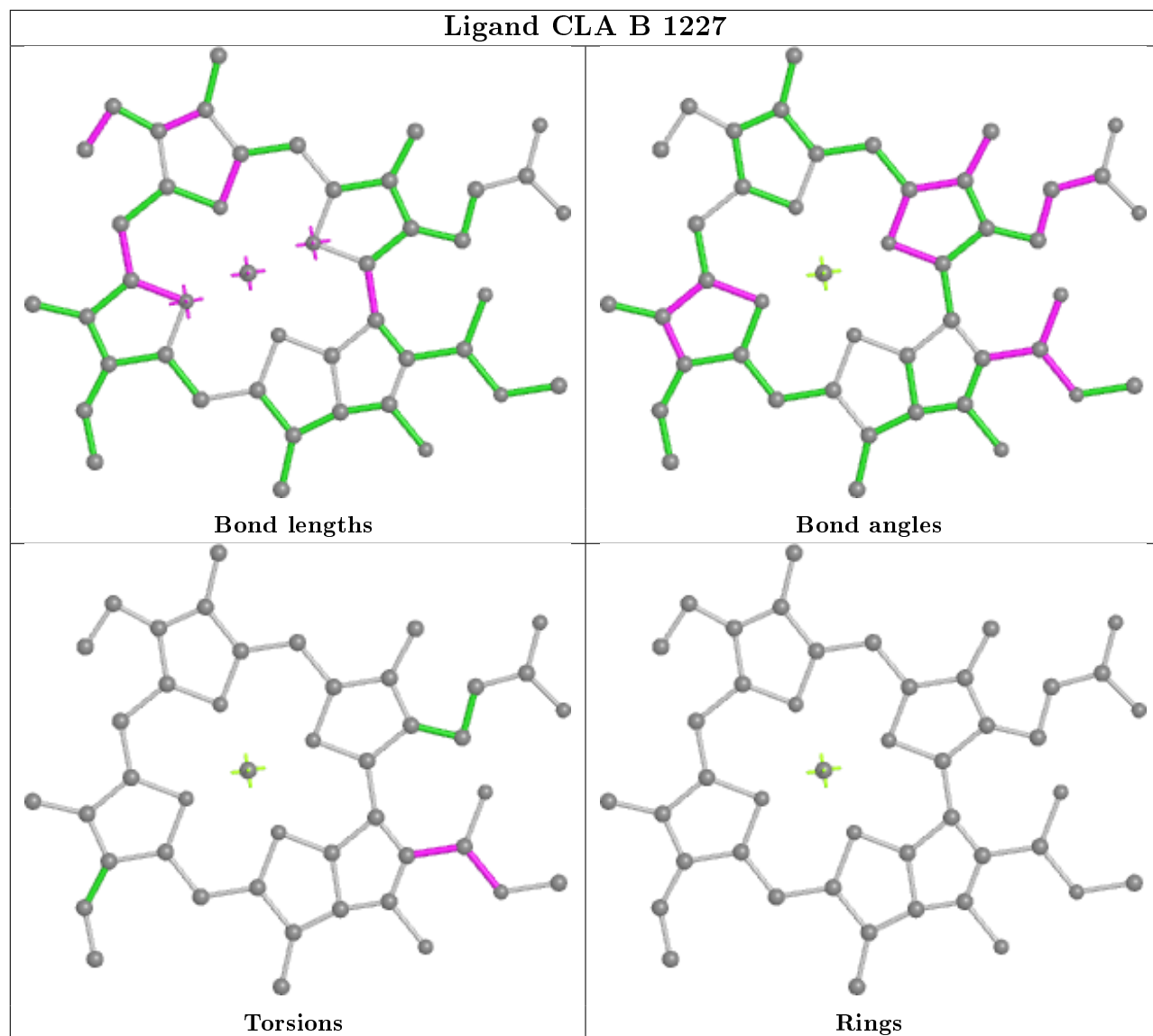
Ligand SQD 1 811



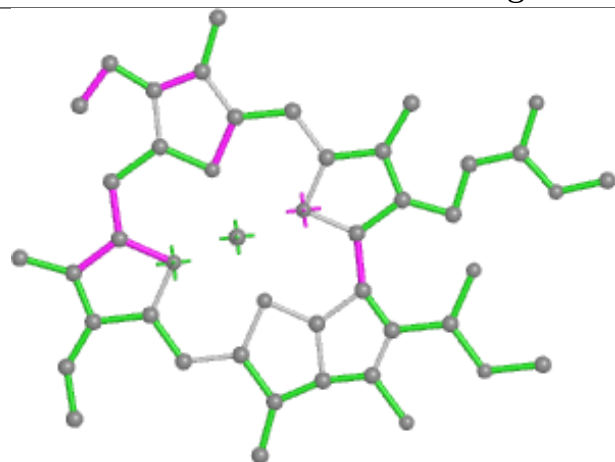
Ligand CLA 1 601



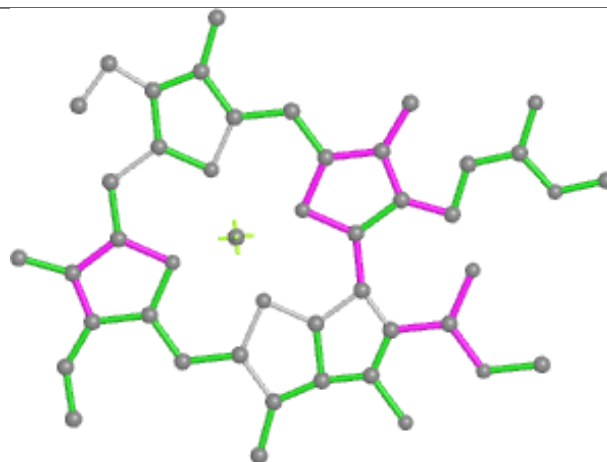
Ligand CLA B 1227



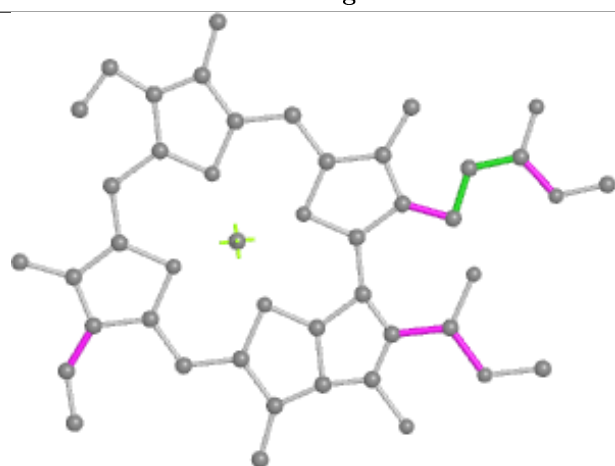
Ligand CLA A 1108



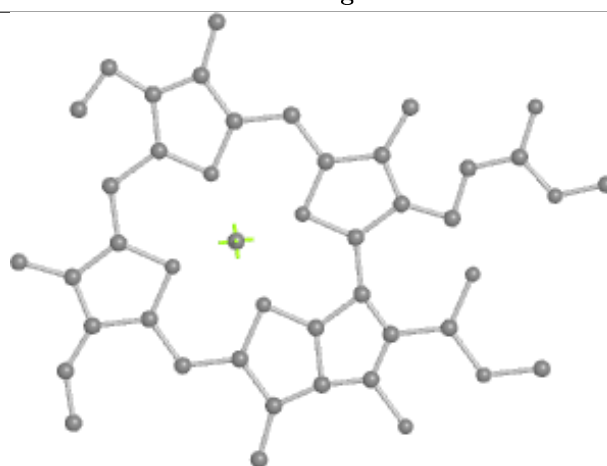
Bond lengths



Bond angles

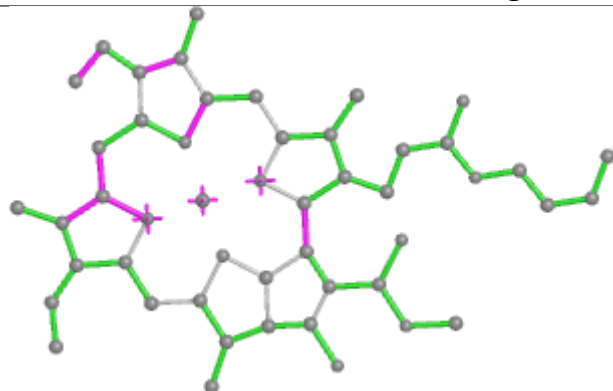


Torsions

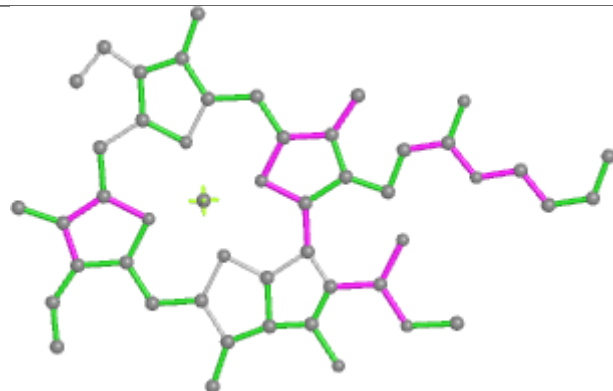


Rings

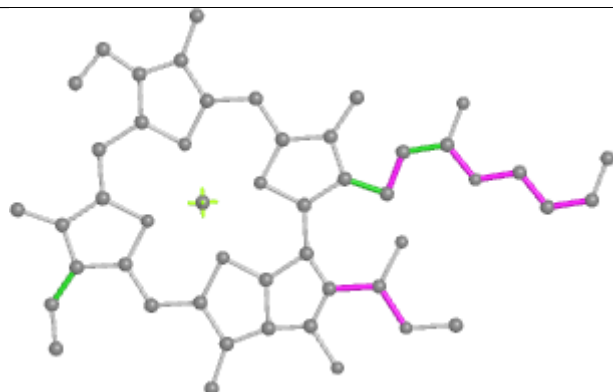
Ligand CLA B 1214



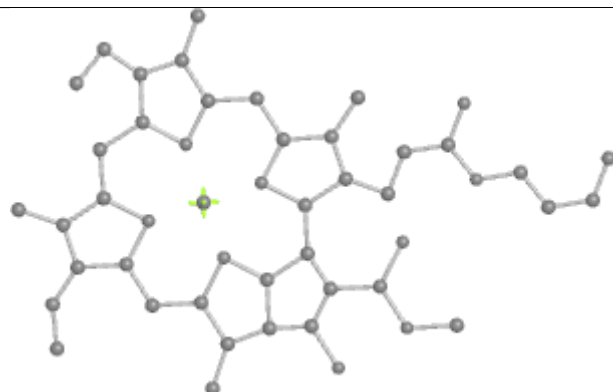
Bond lengths



Bond angles

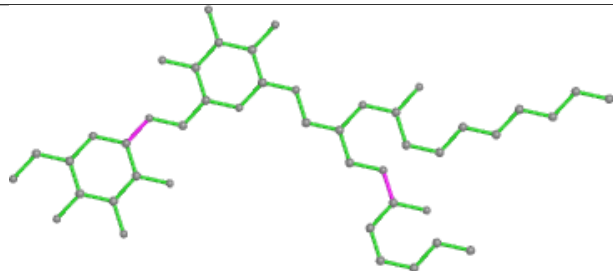


Torsions

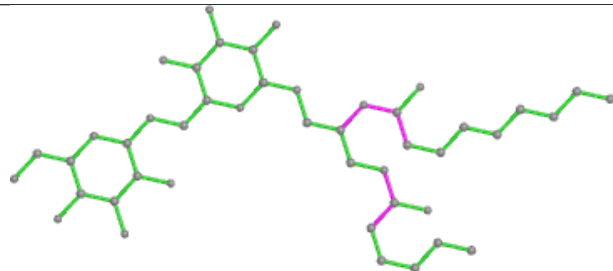


Rings

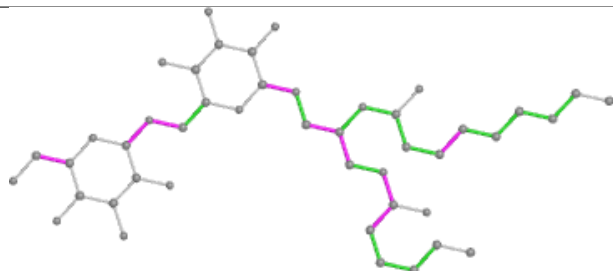
Ligand DGD 4 811



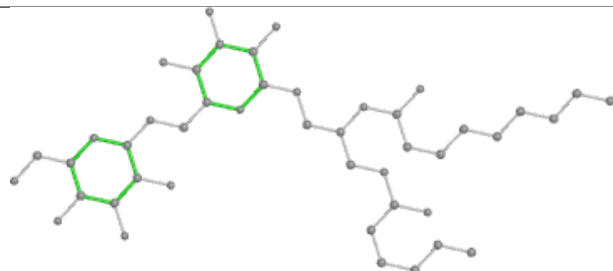
Bond lengths



Bond angles

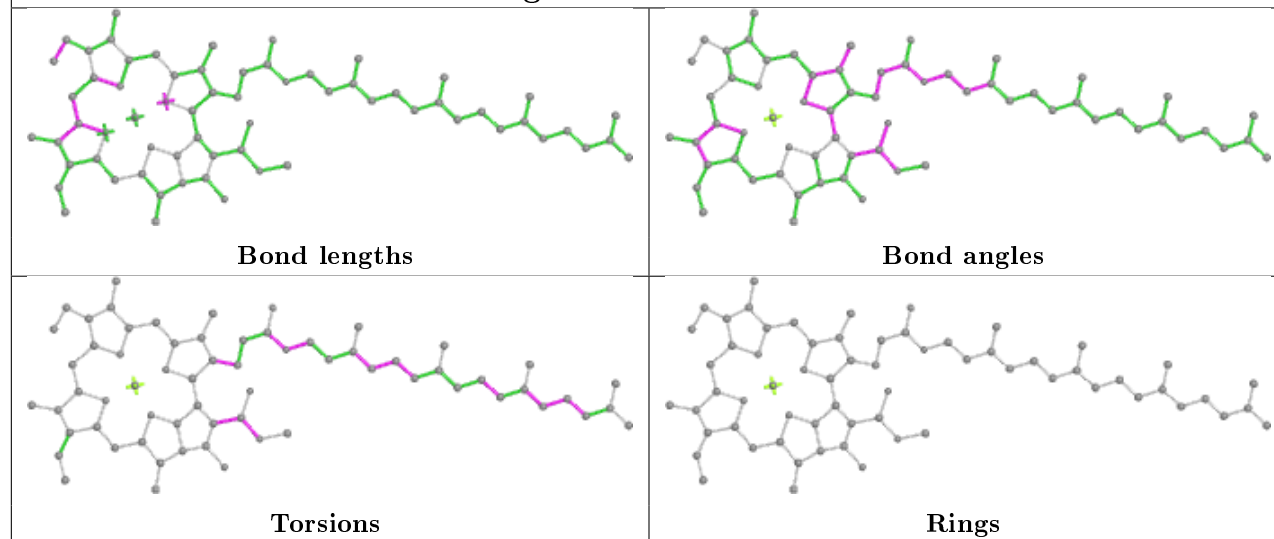


Torsions

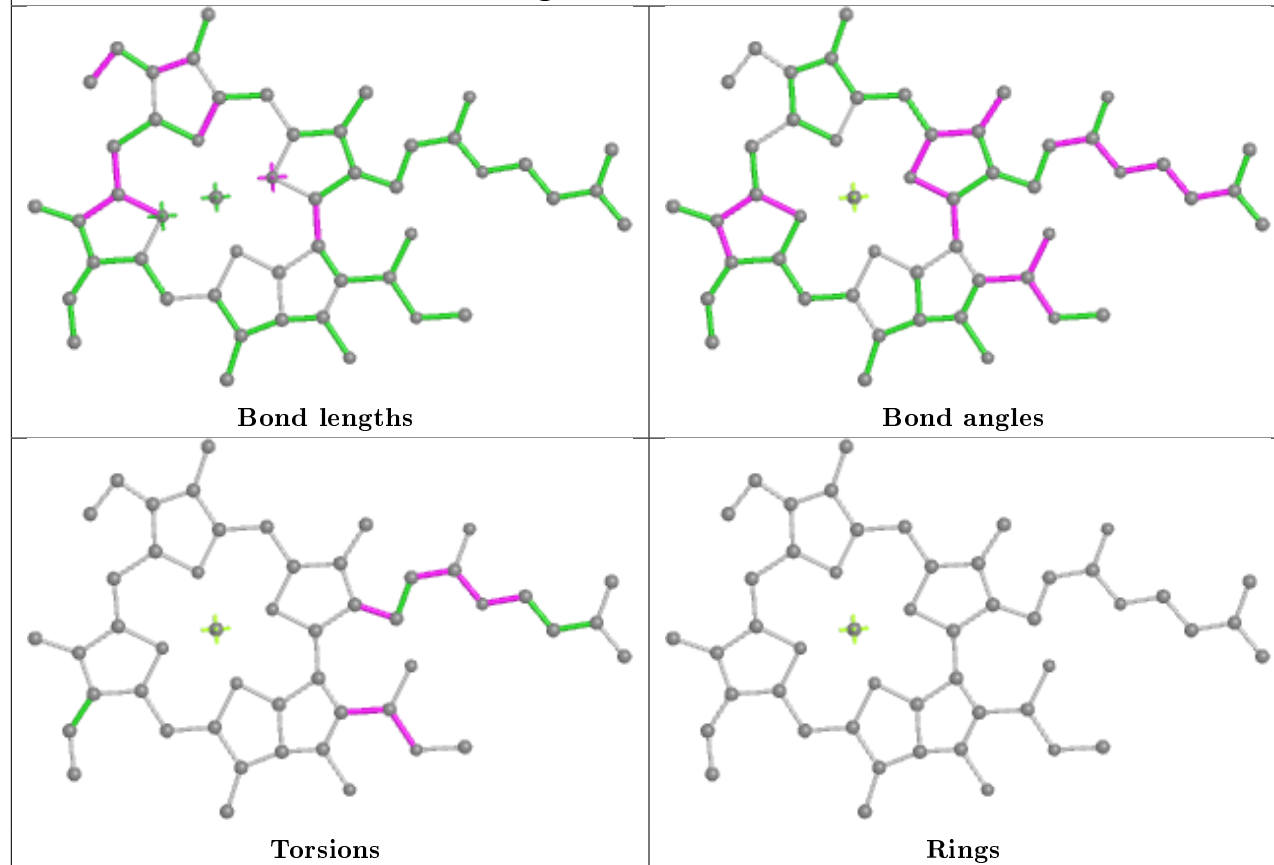


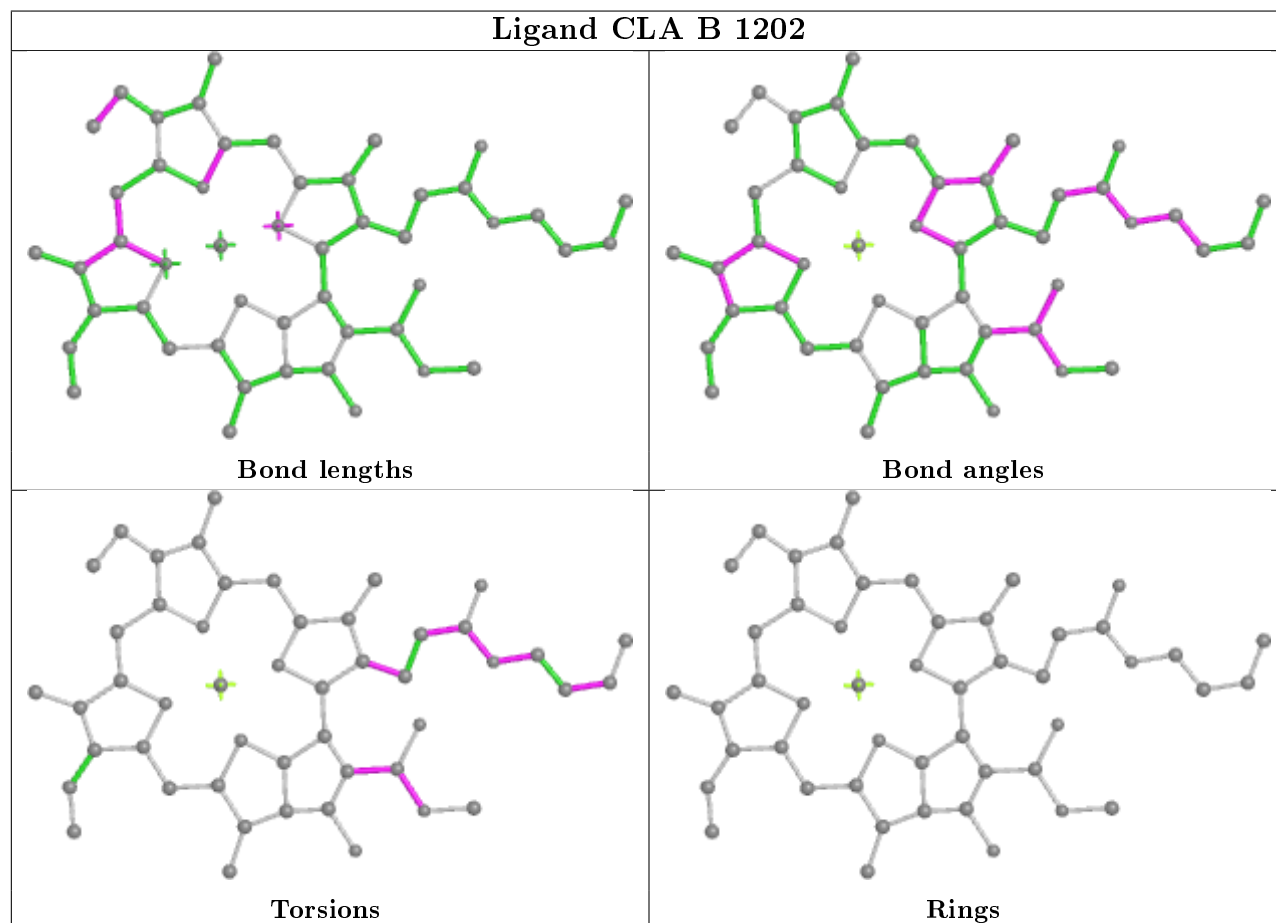
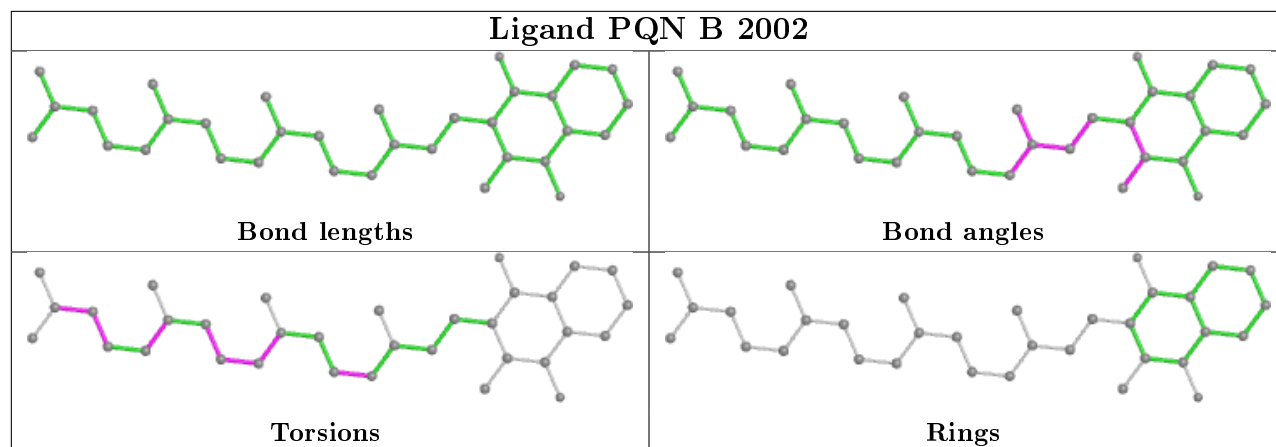
Rings

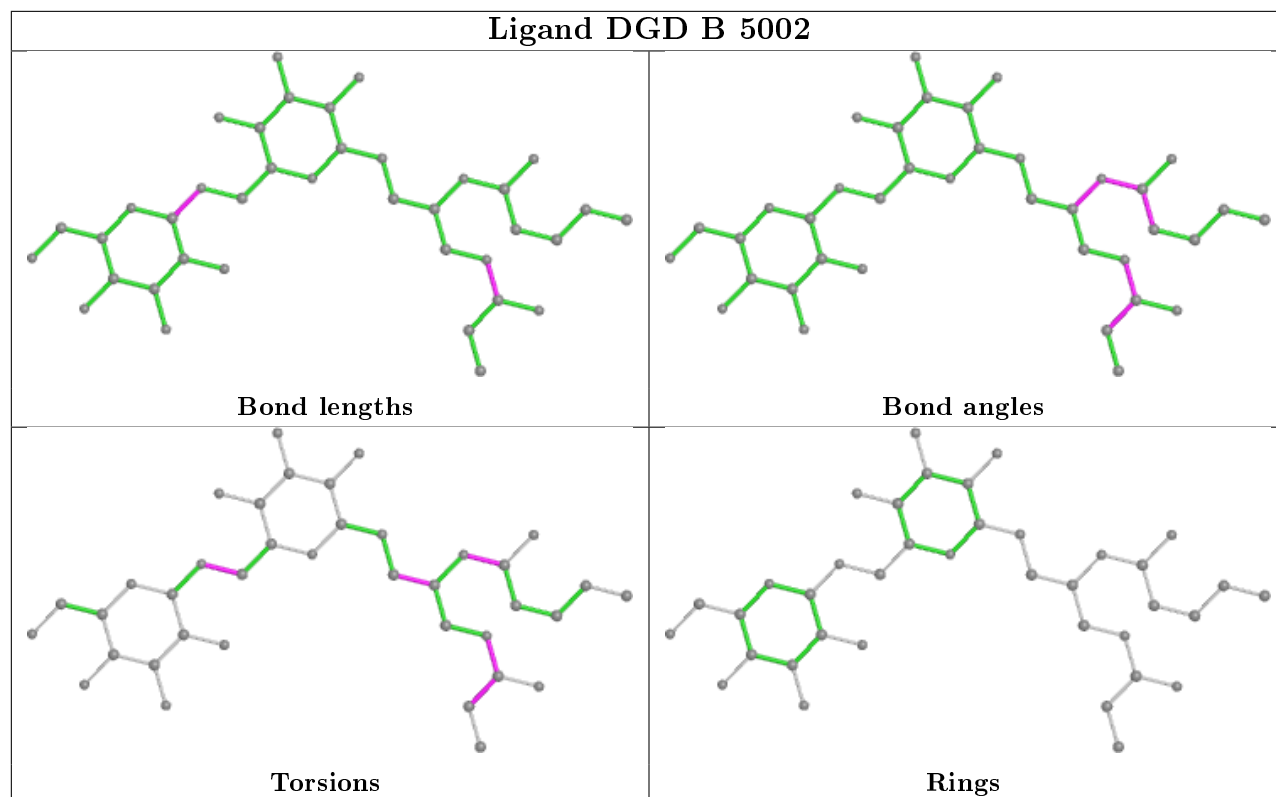
Ligand CLA B 1229



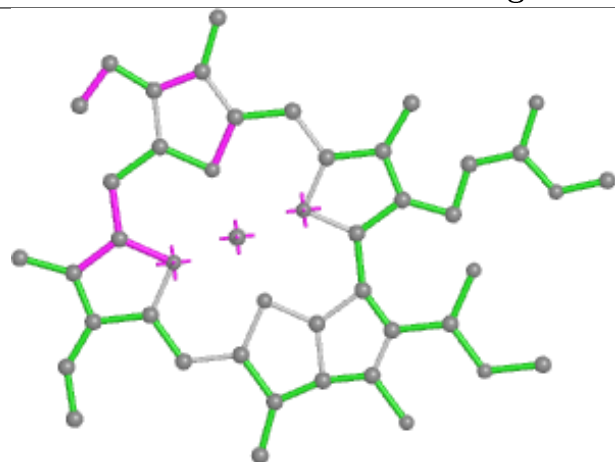
Ligand CLA 3 607



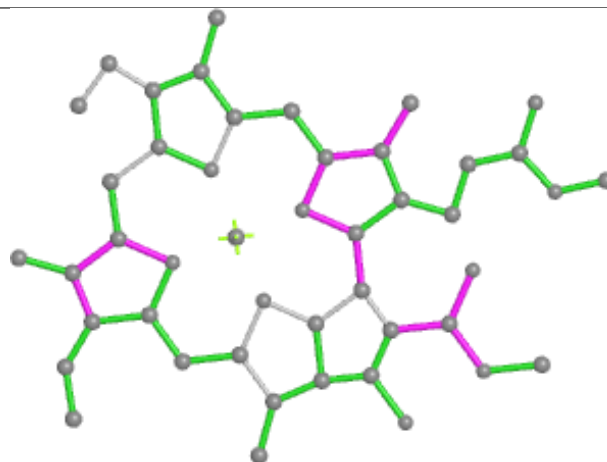




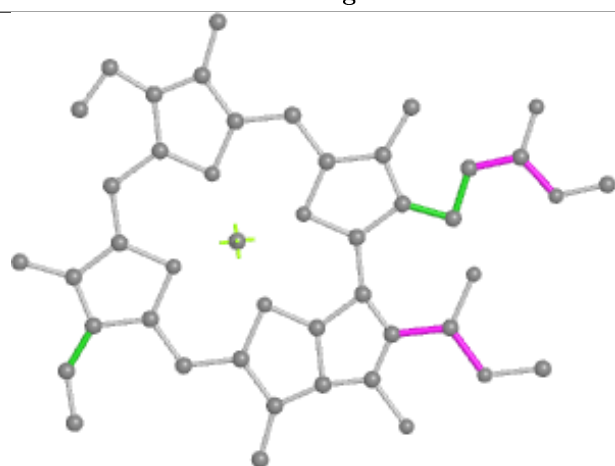
Ligand CLA B 1209



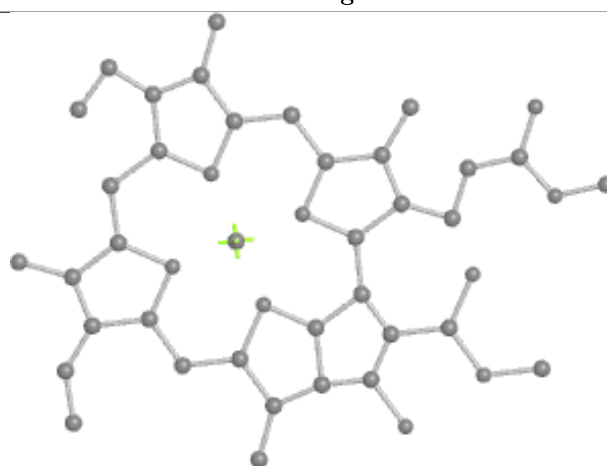
Bond lengths



Bond angles

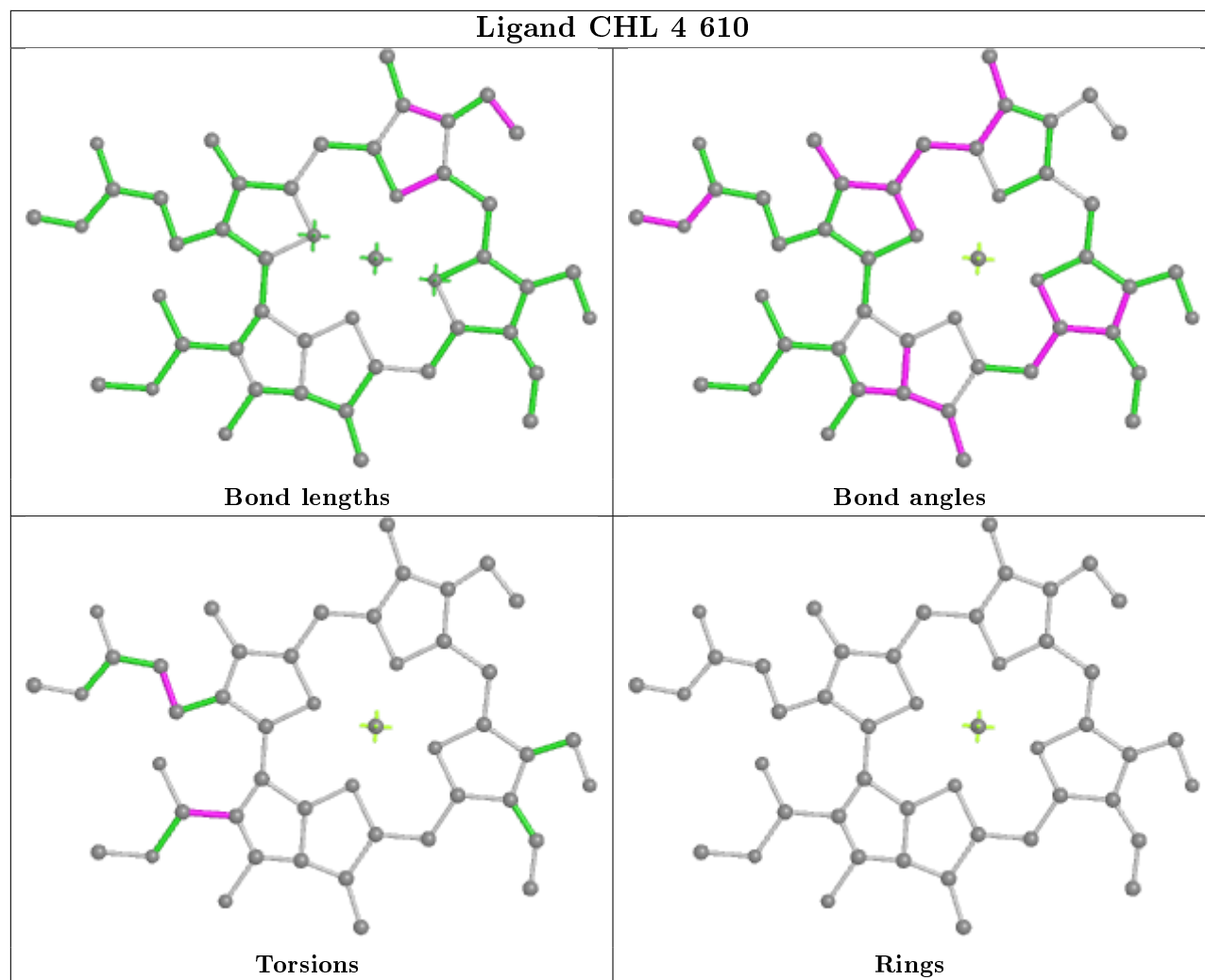


Torsions

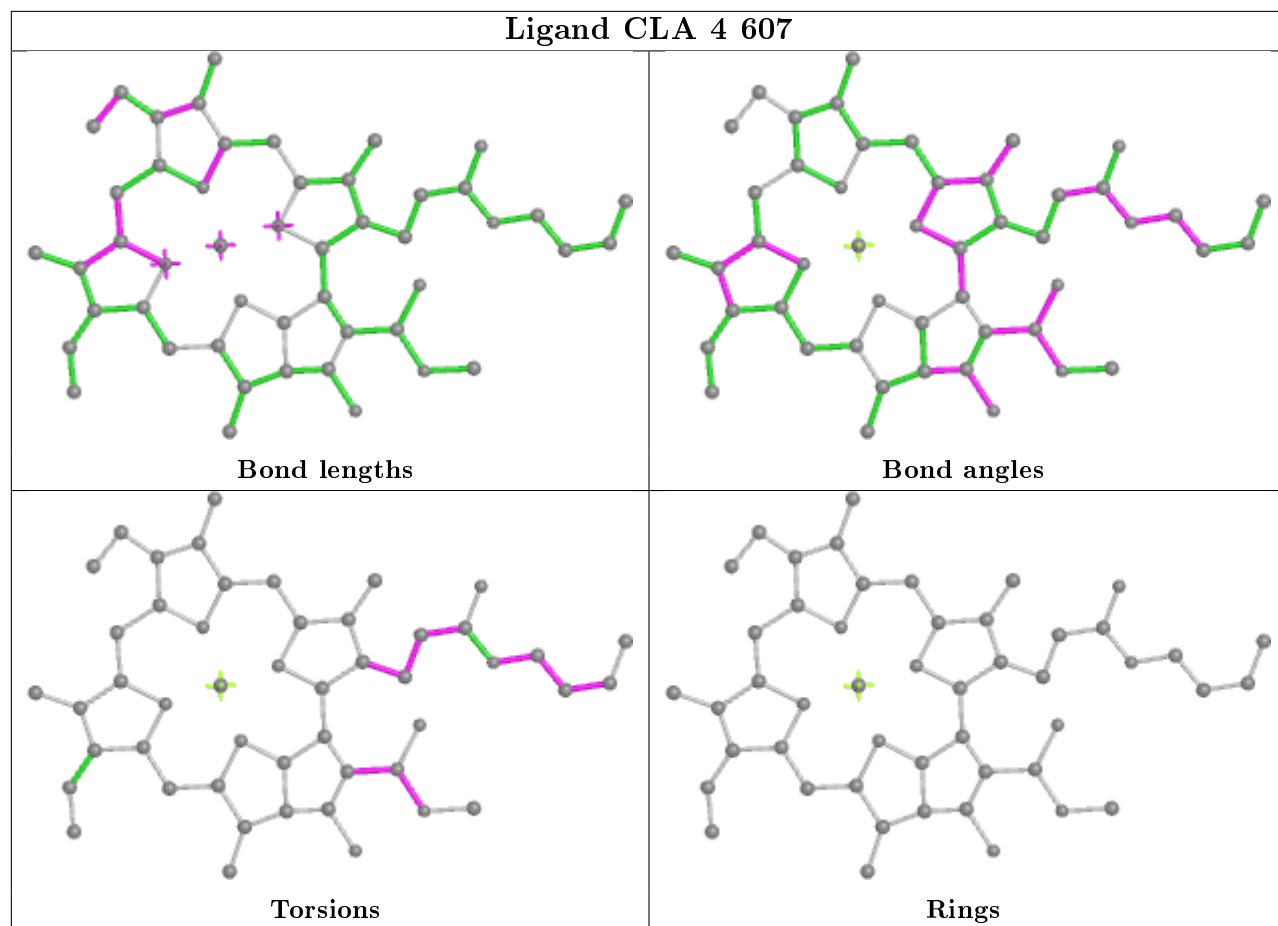


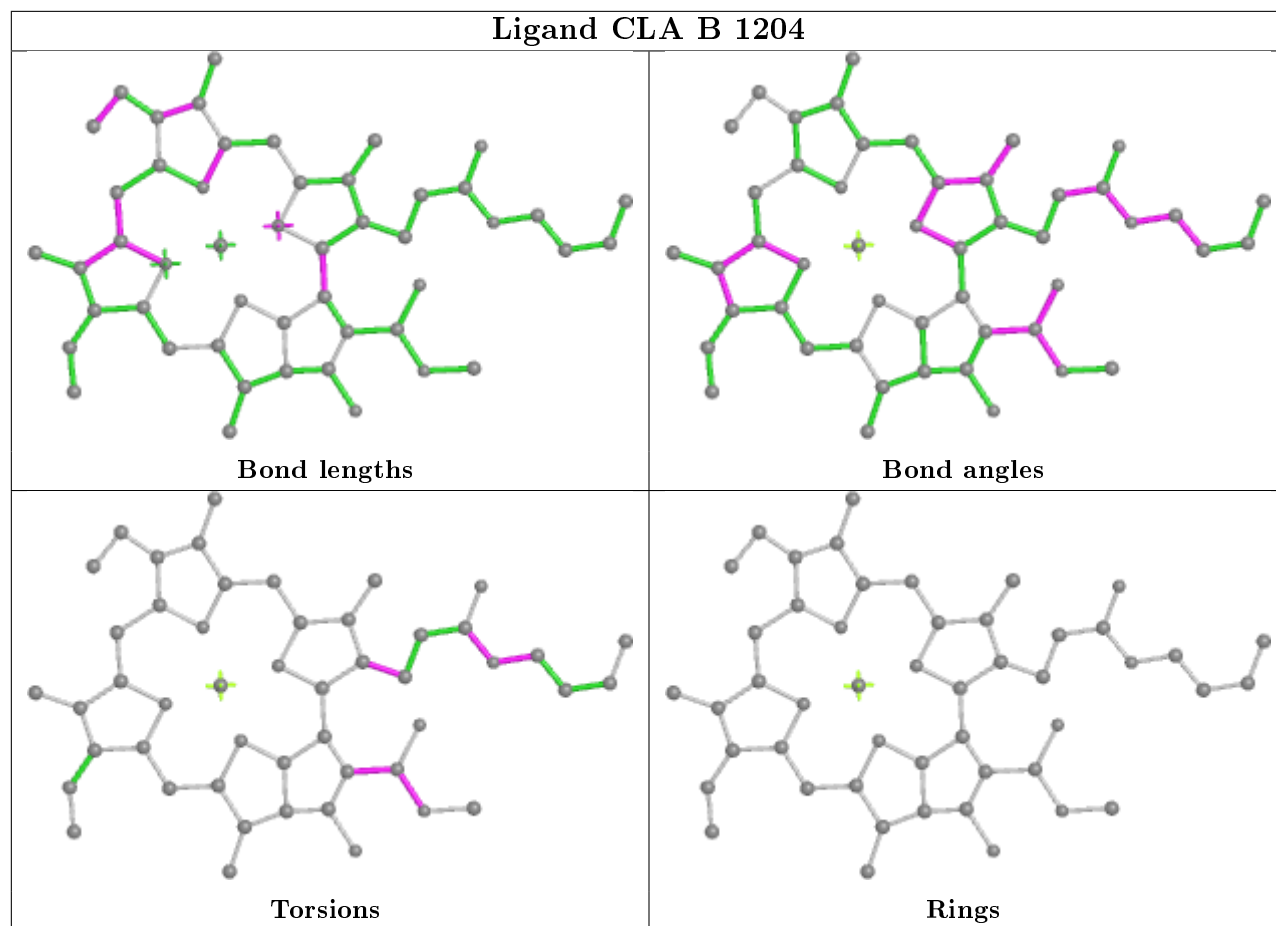
Rings

Ligand CHL 4 610

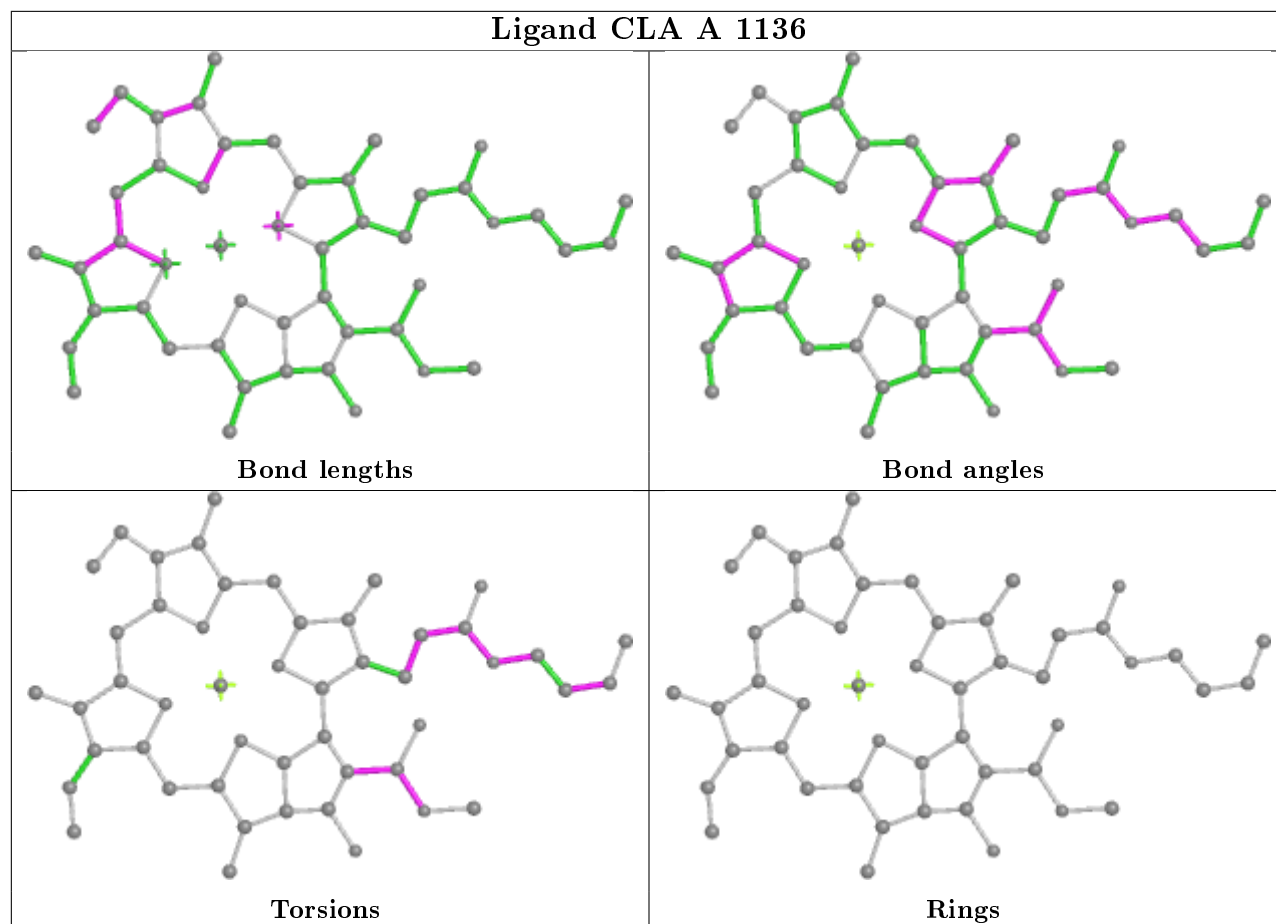


Ligand CLA 4 607

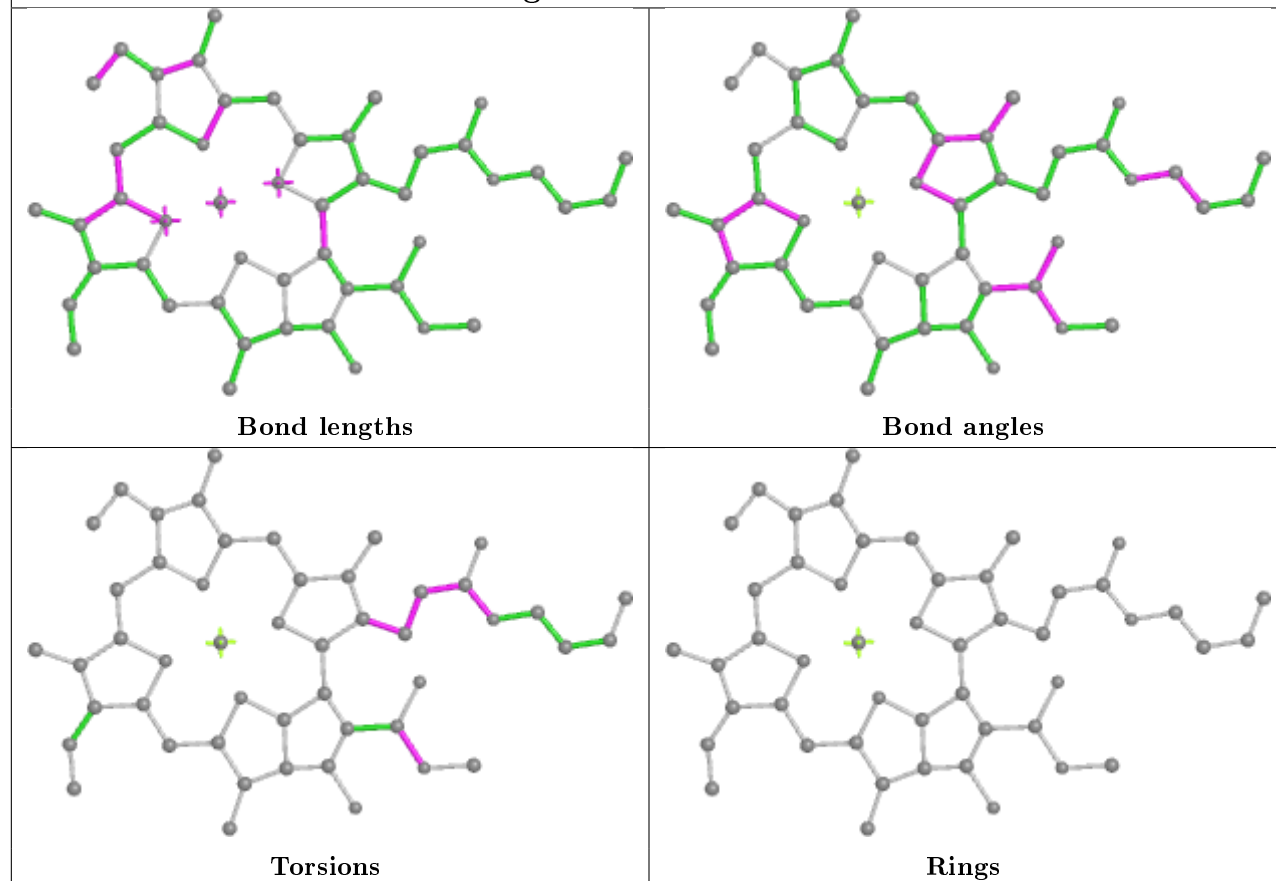




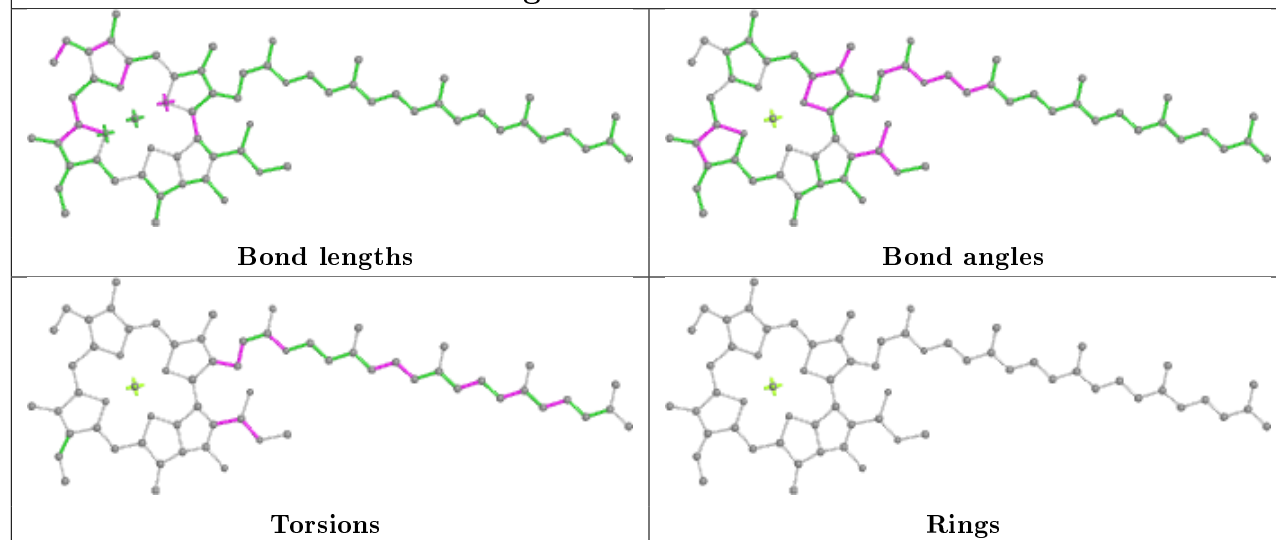
Ligand CLA A 1136



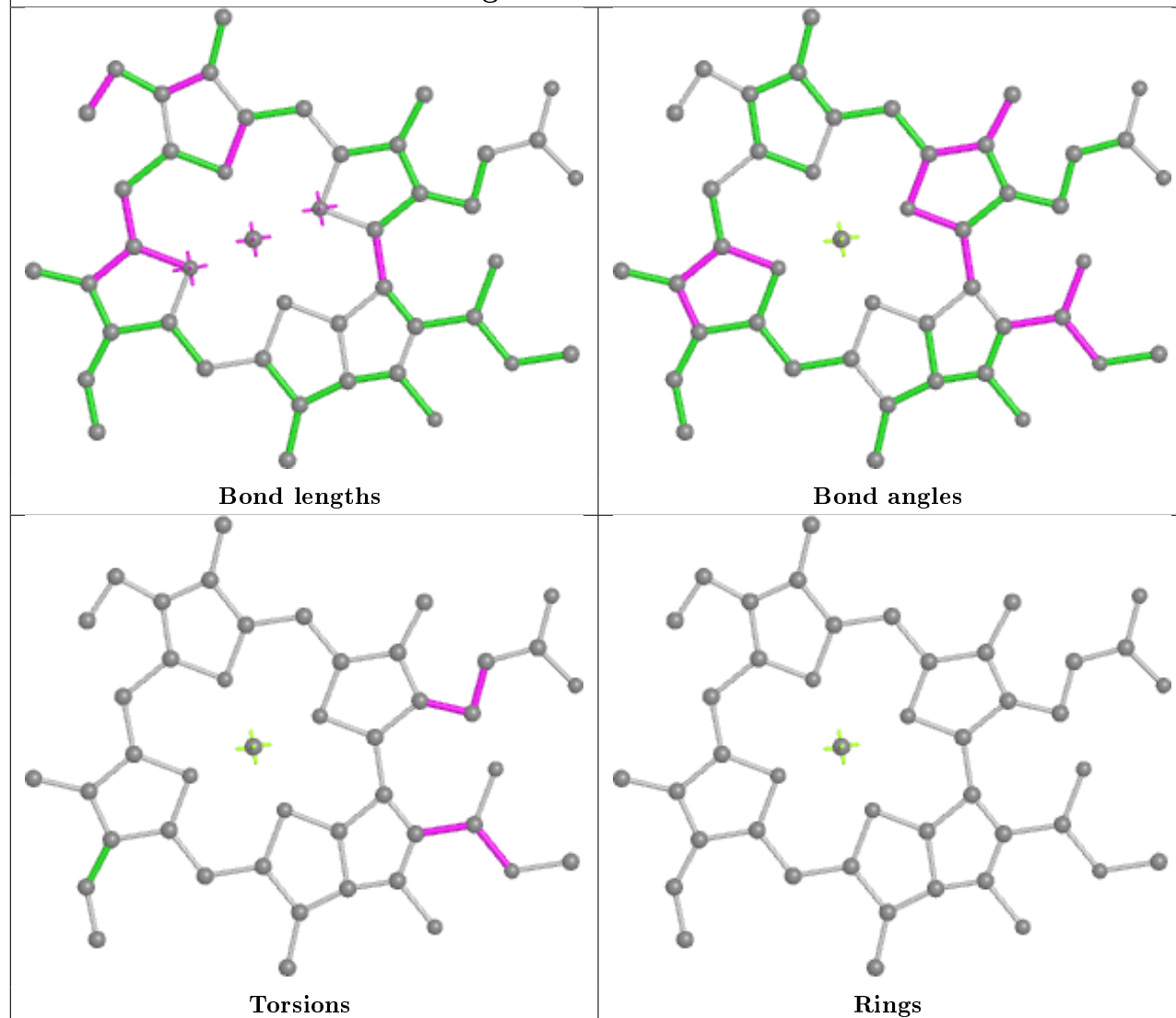
Ligand CLA B 1211



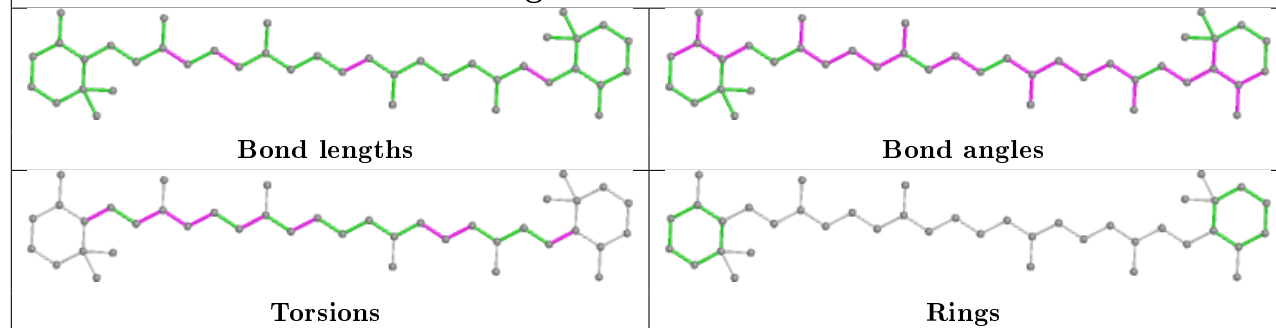
Ligand CLA A 1106



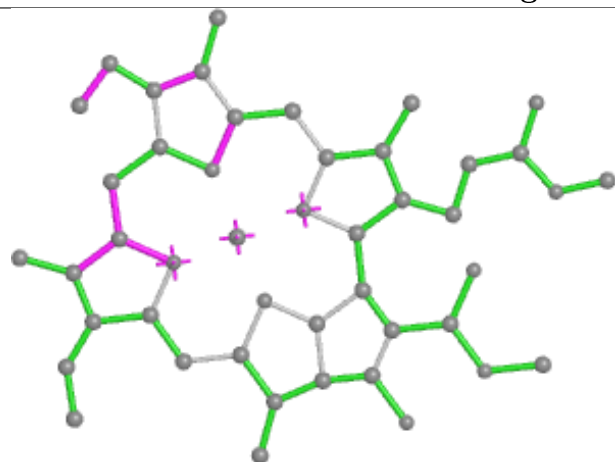
Ligand CLA A 1113



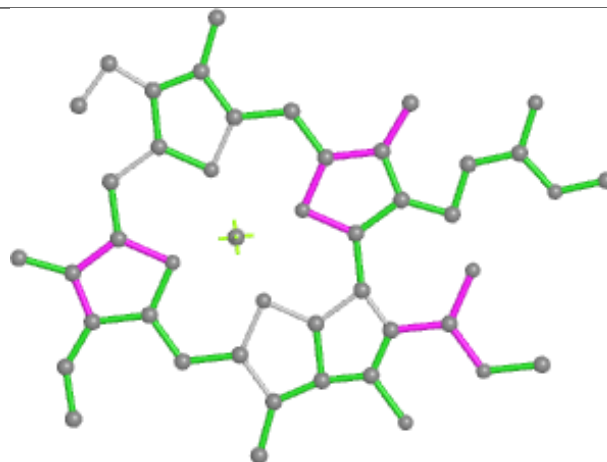
Ligand BCR J 4003



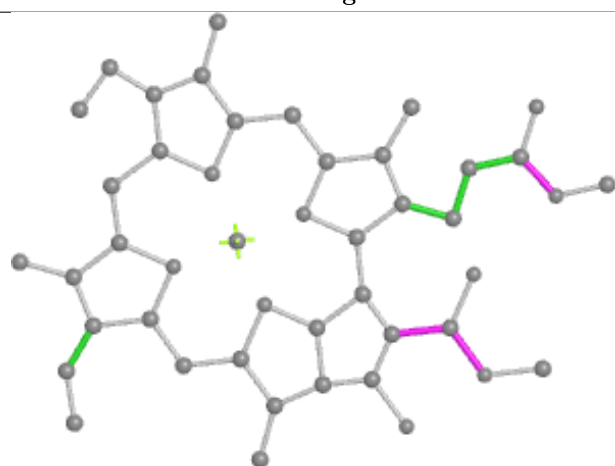
Ligand CLA 4 608



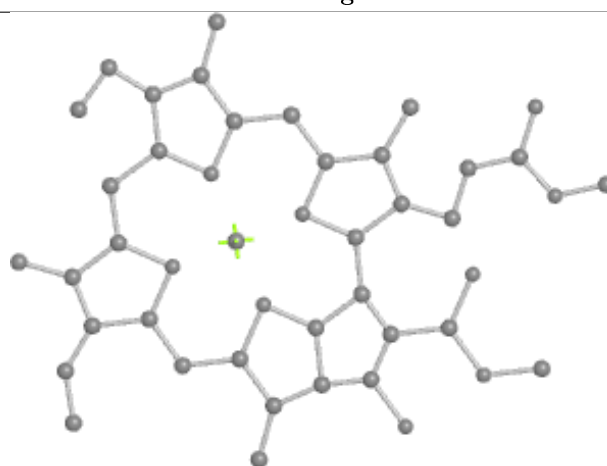
Bond lengths



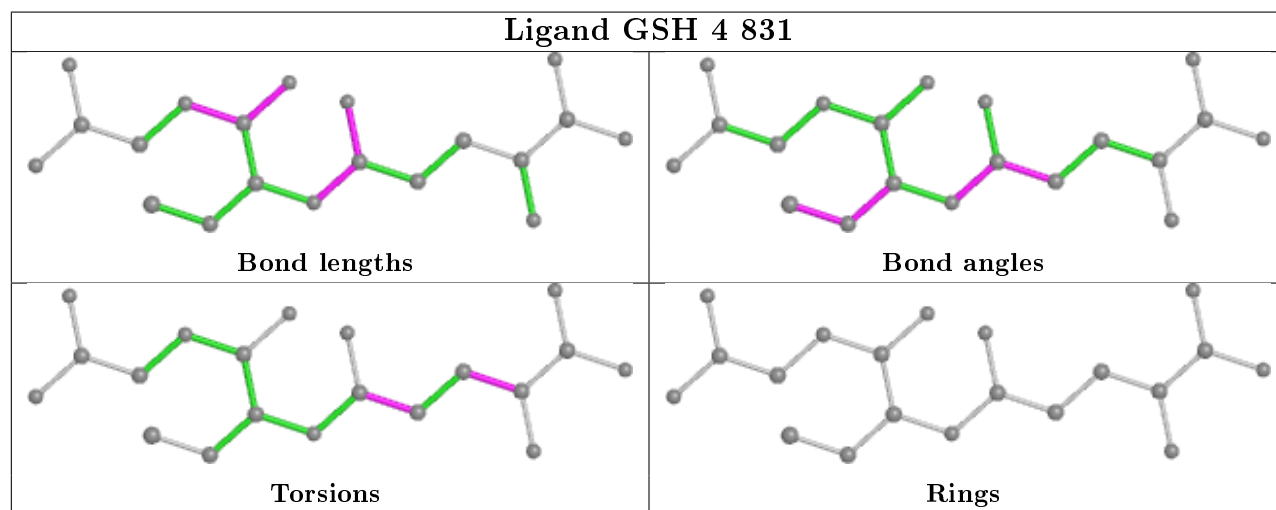
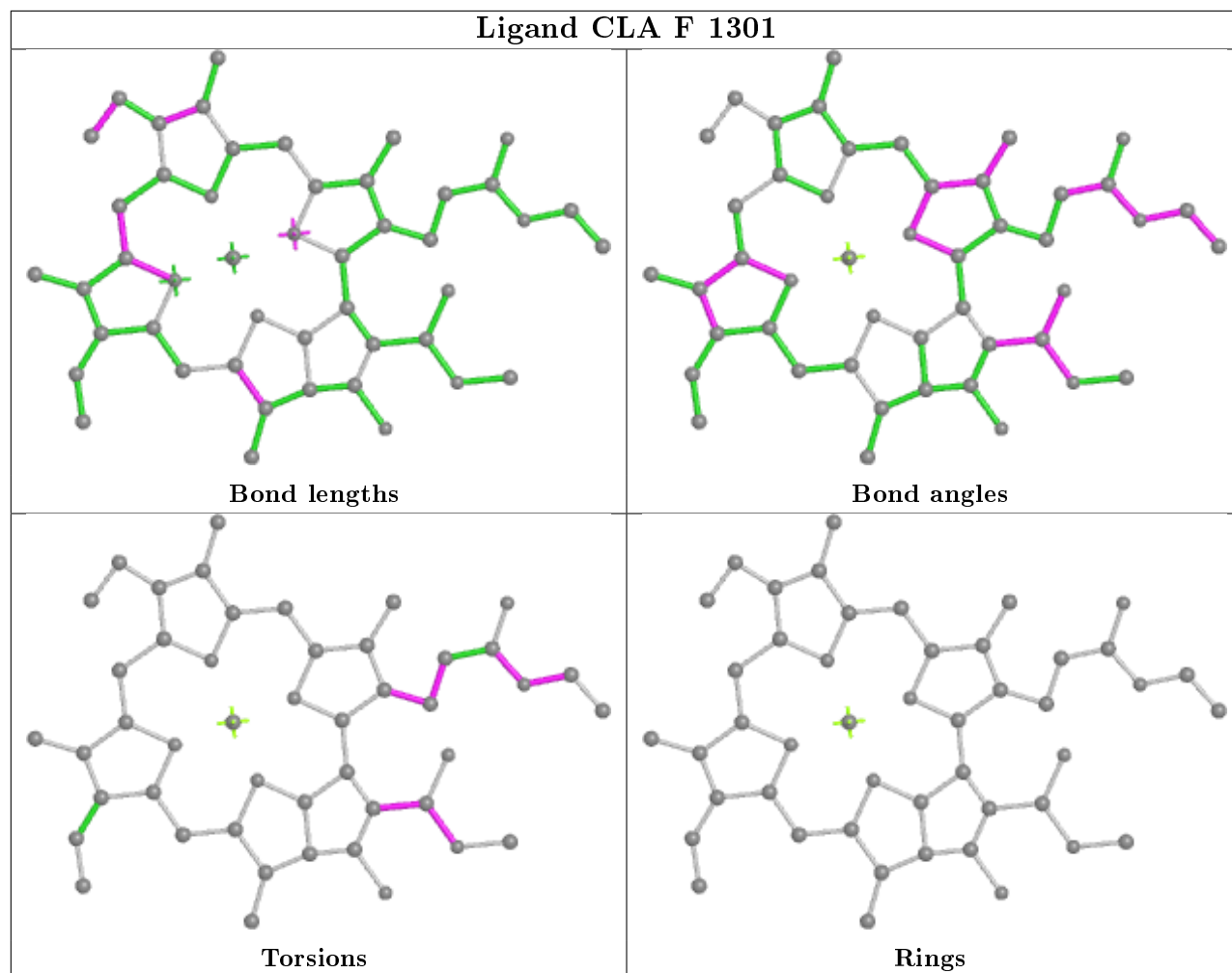
Bond angles

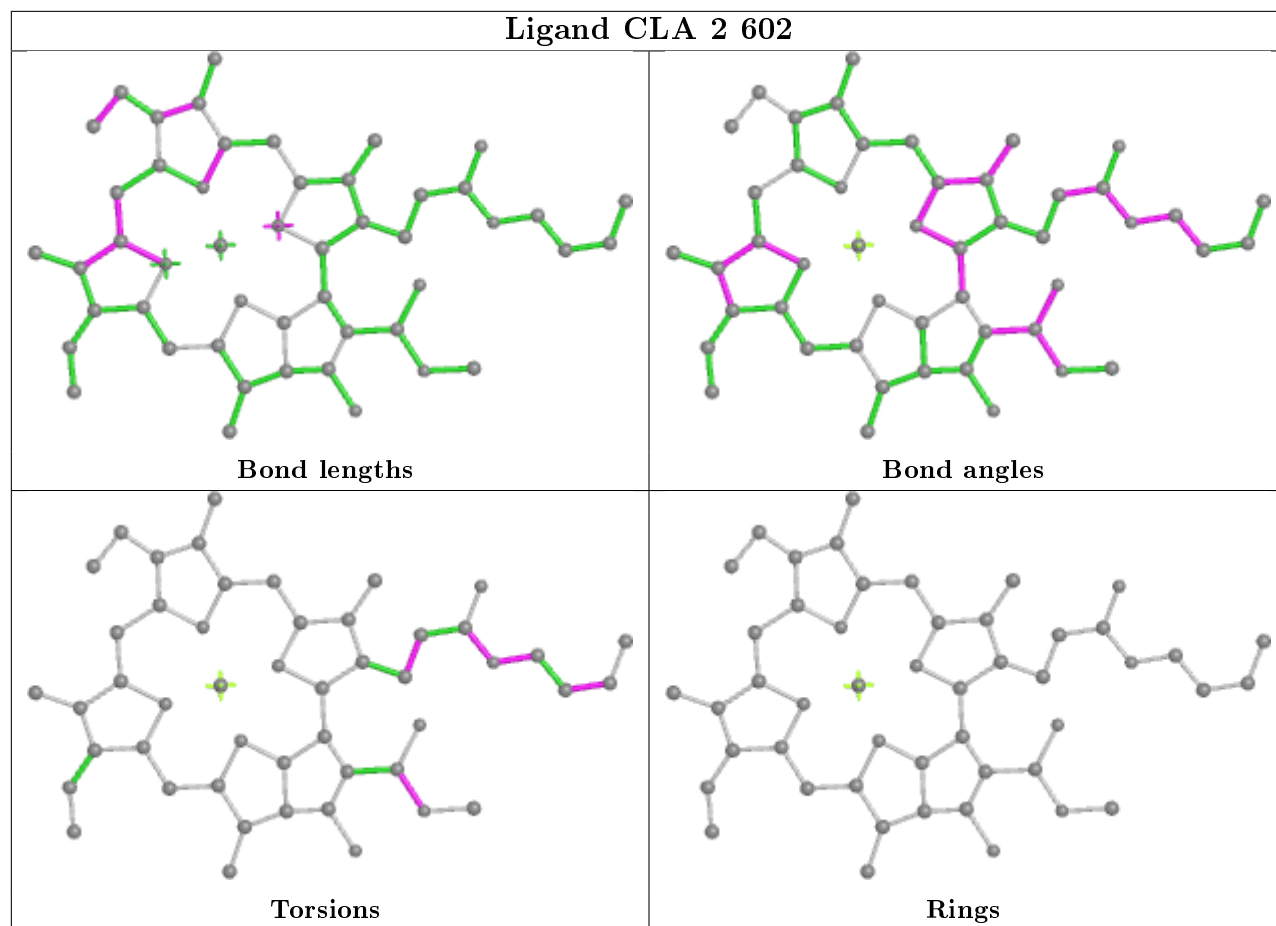


Torsions

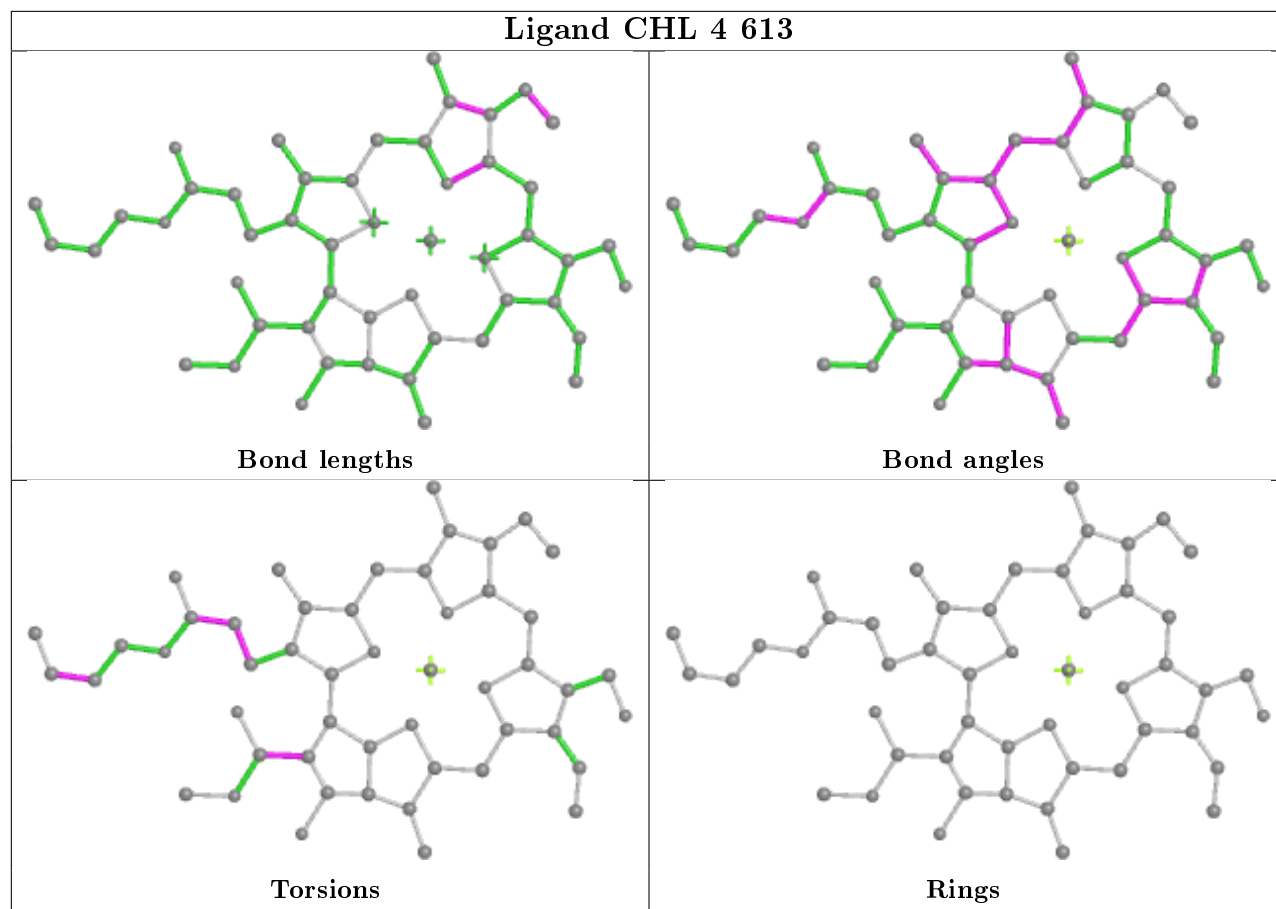


Rings

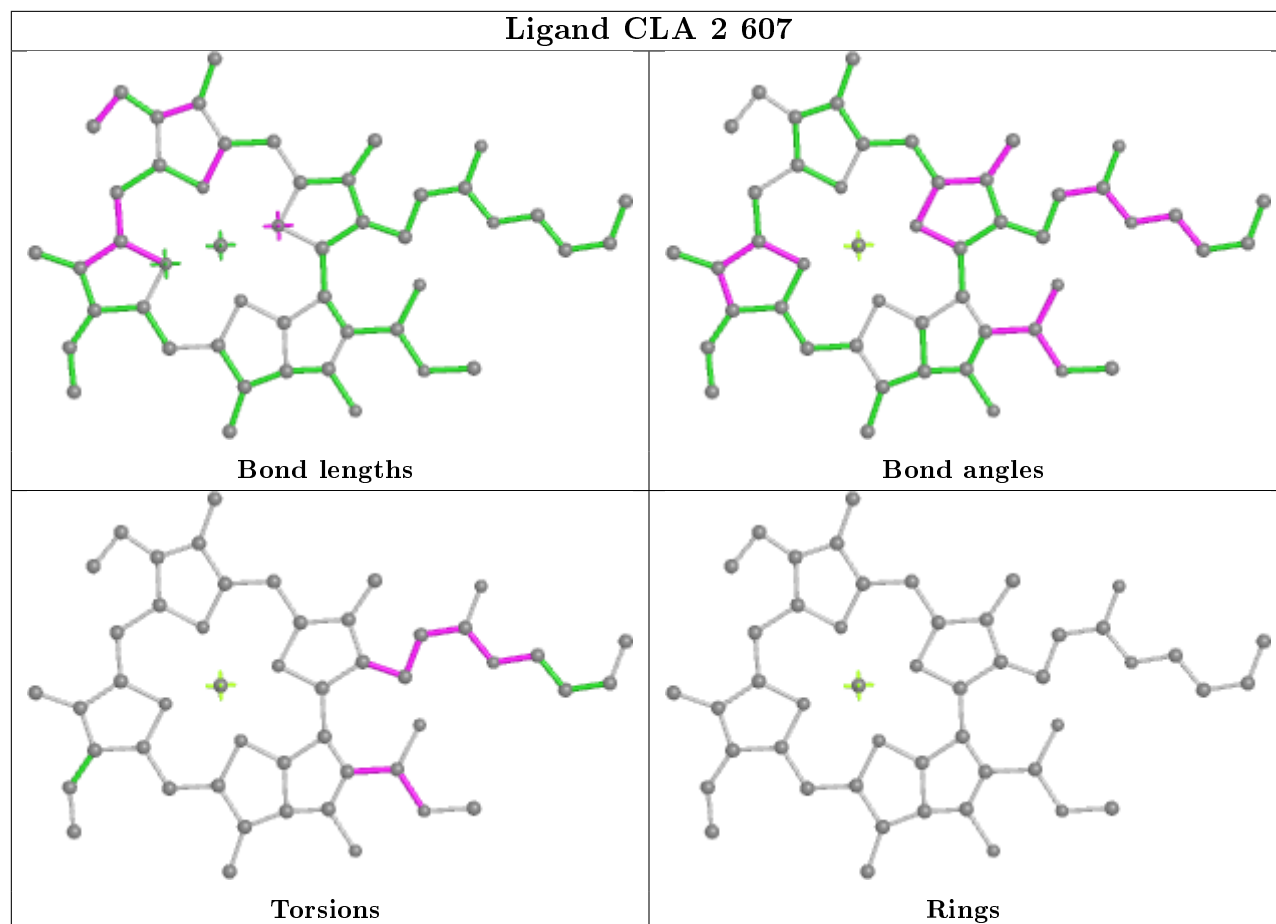


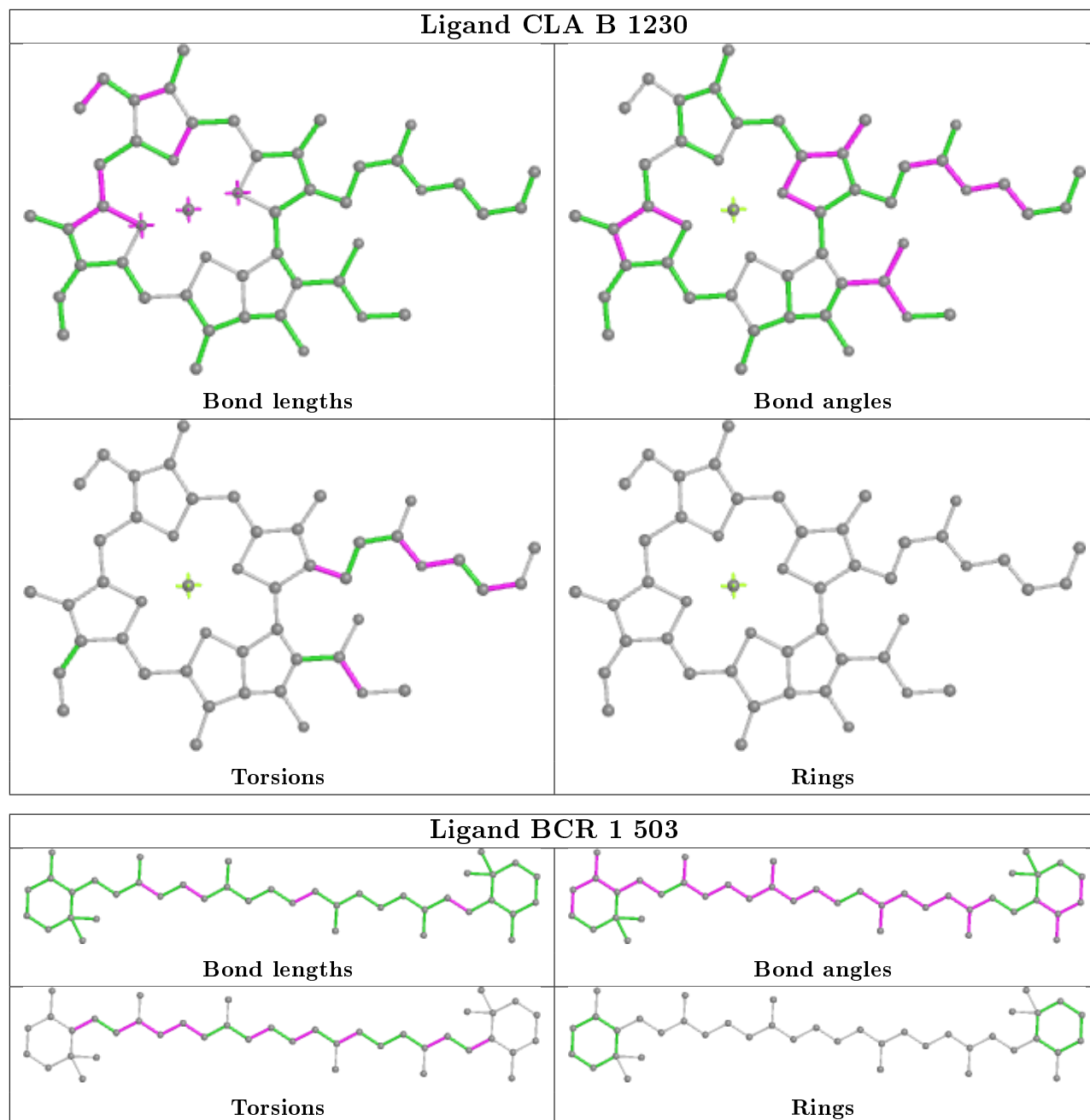


Ligand CHL 4 613

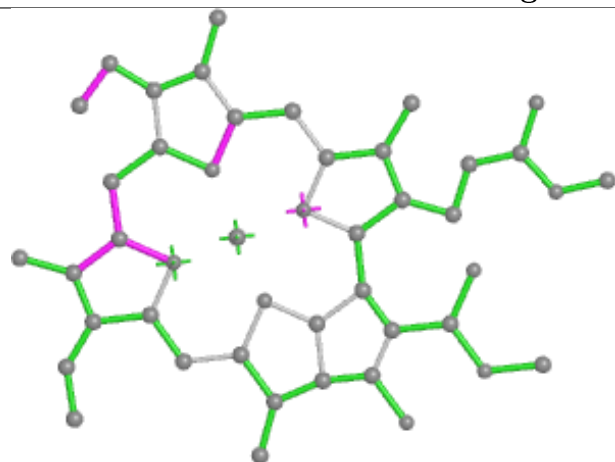


Ligand CLA 2 607

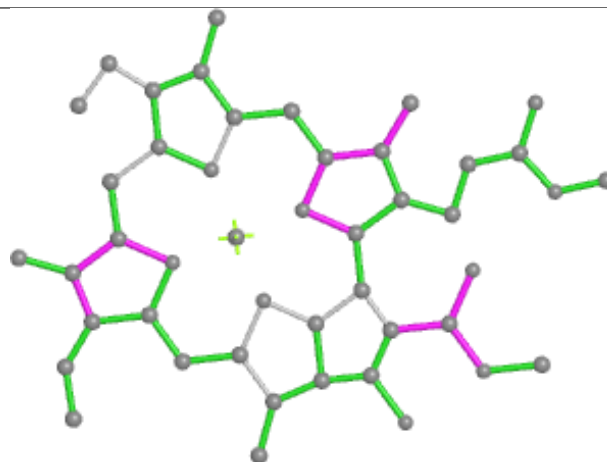




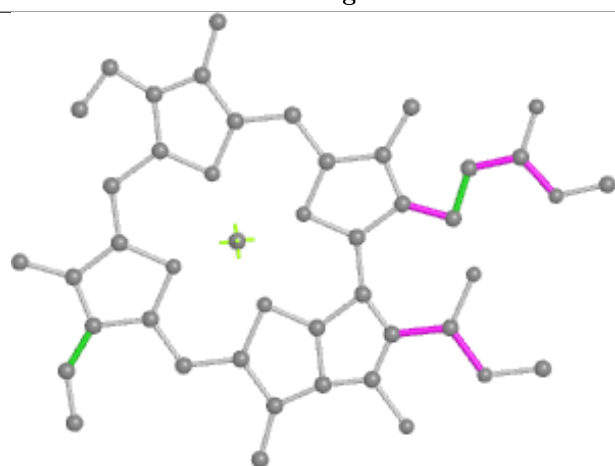
Ligand CLA 3 613



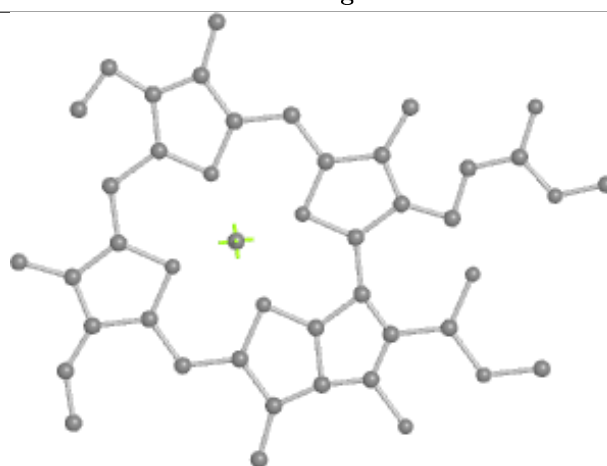
Bond lengths



Bond angles

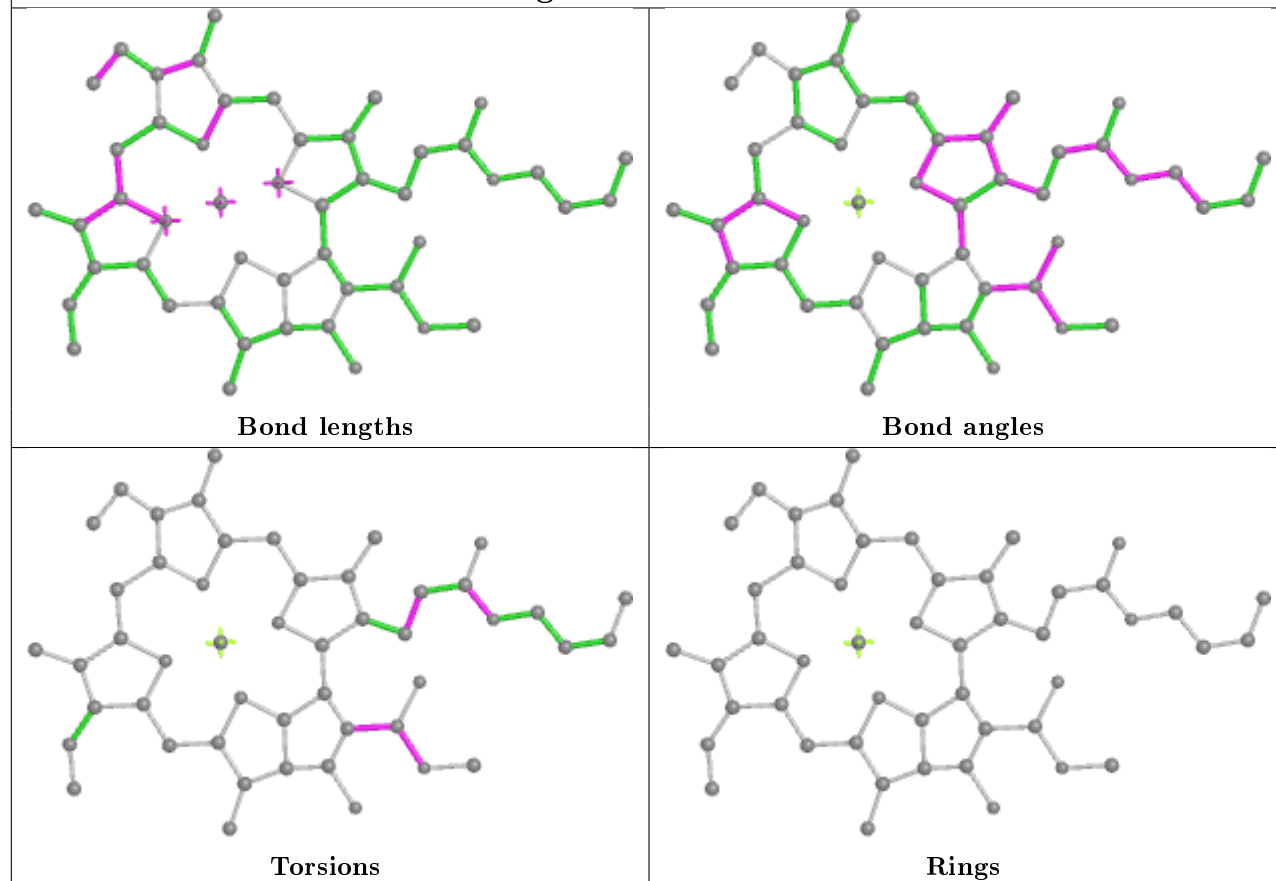


Torsions

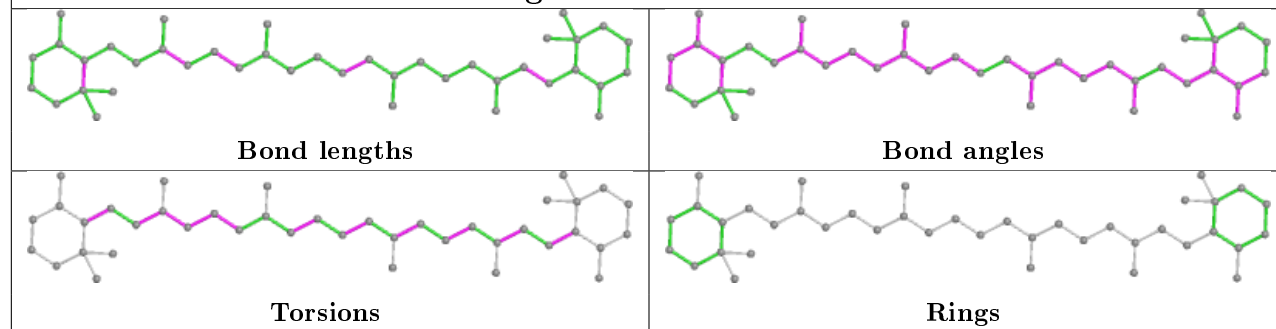


Rings

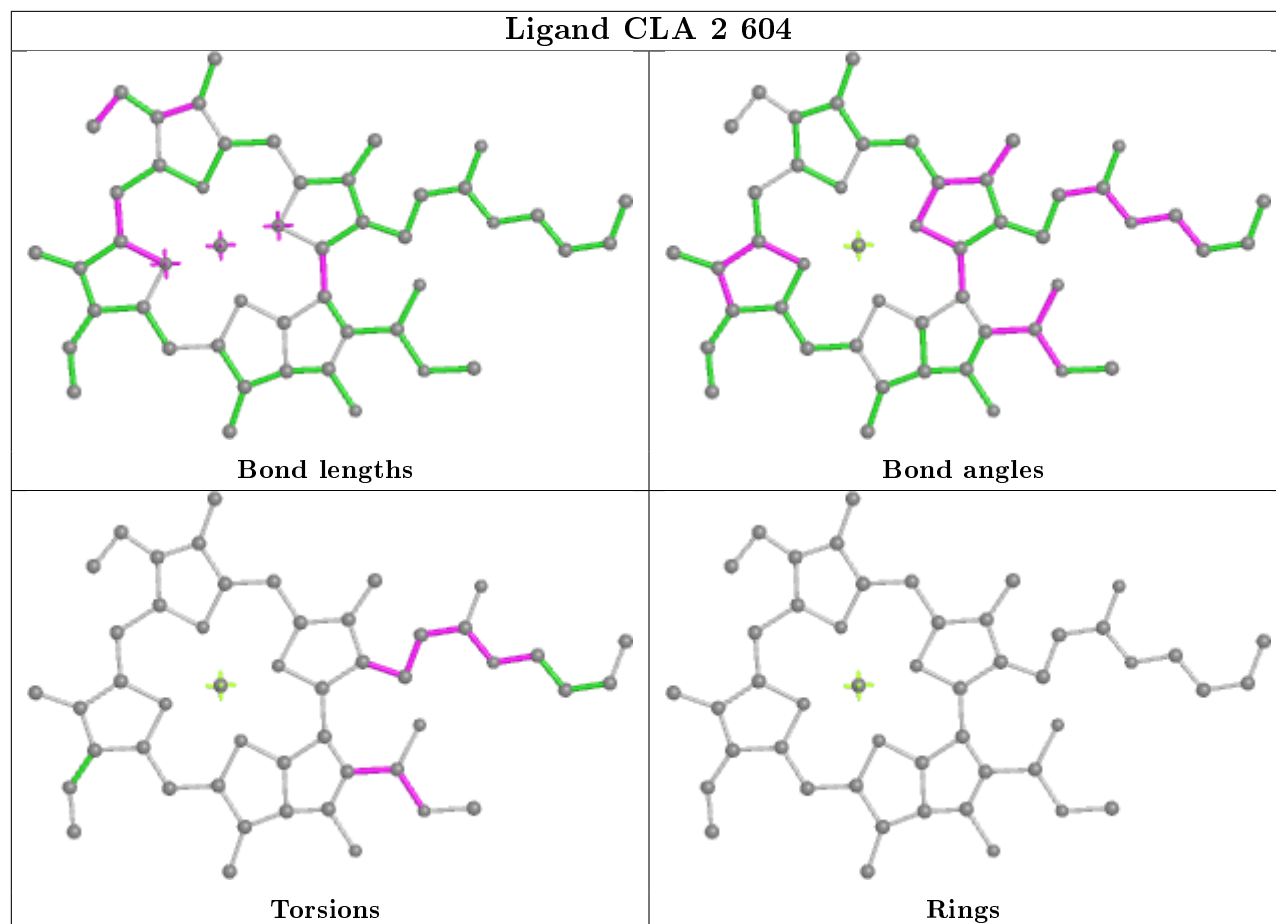
Ligand CLA 1 604



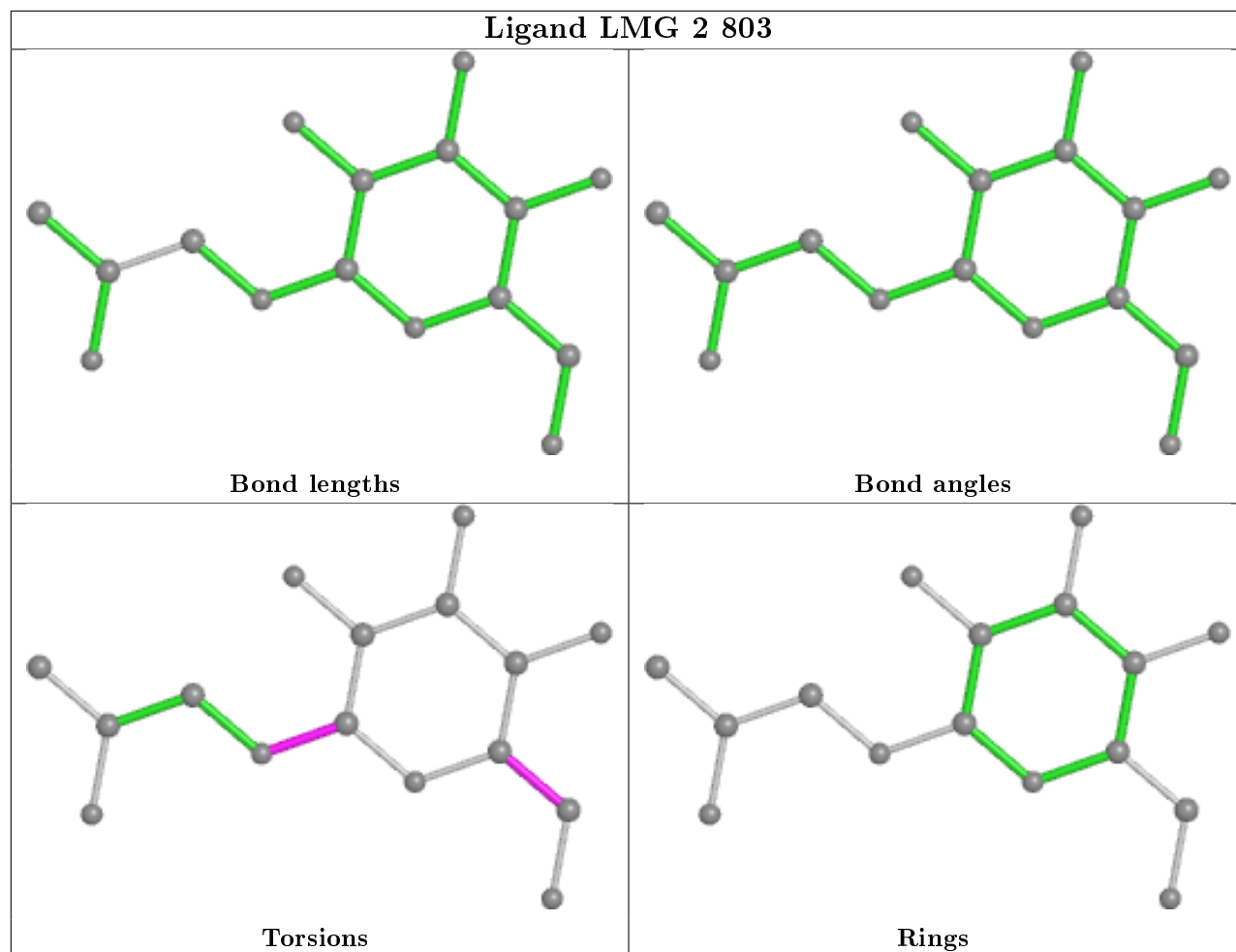
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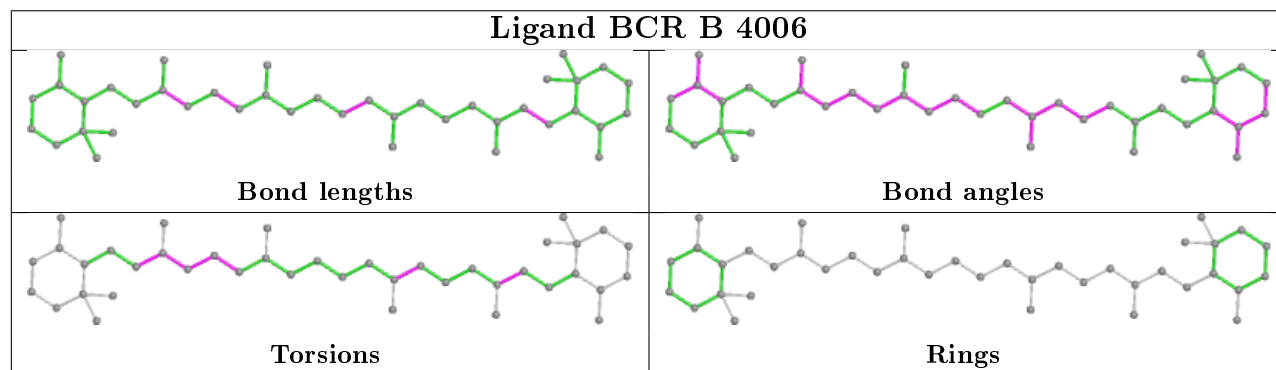
Ligand CLA 2 604



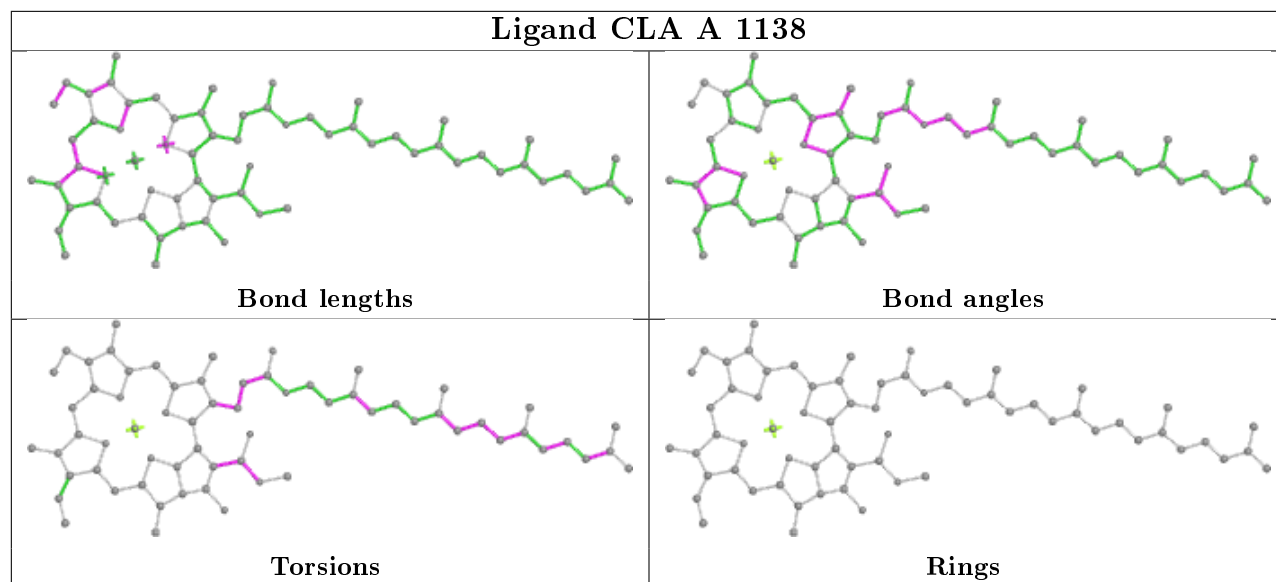
Ligand LMG 2 803



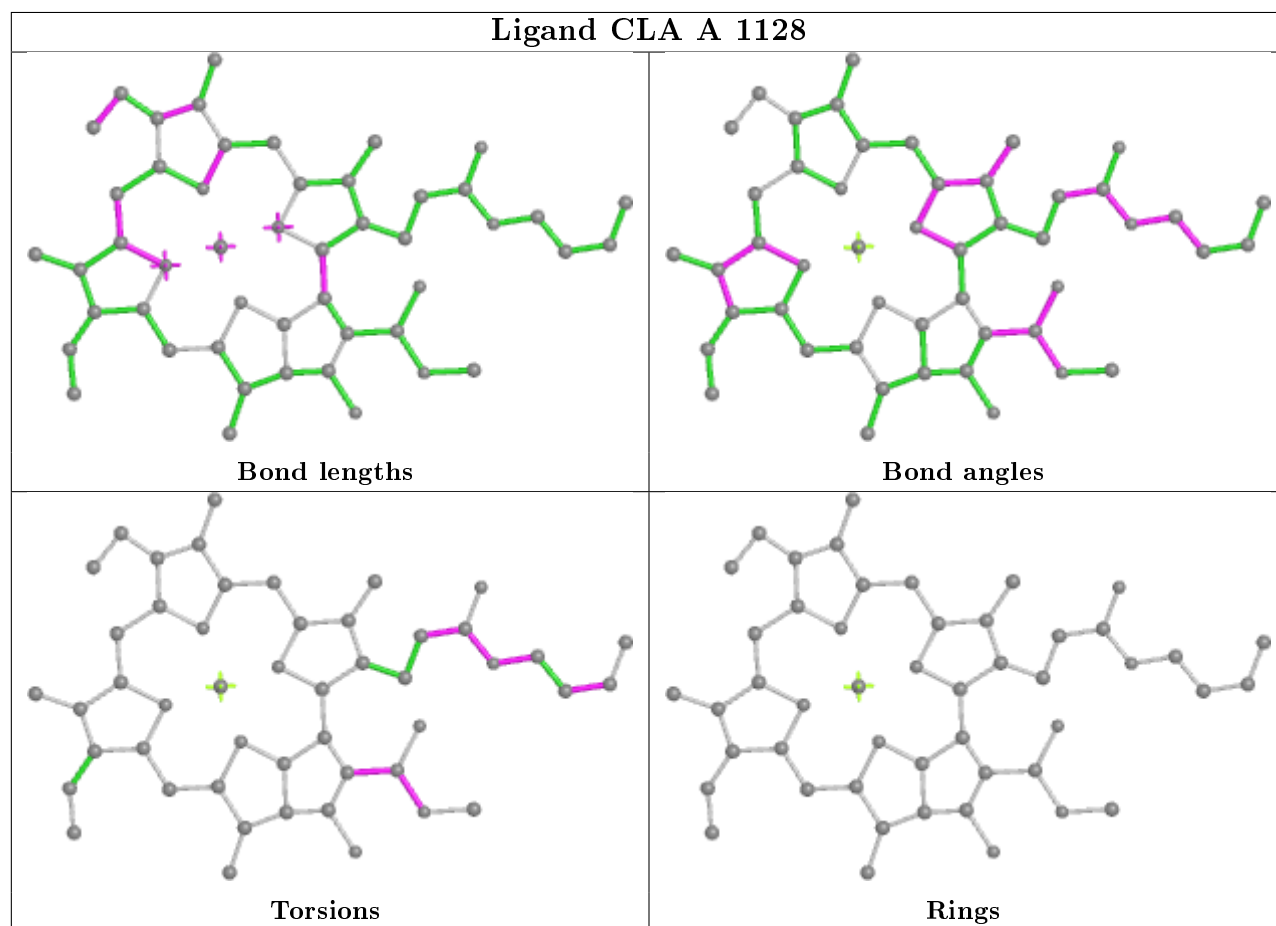
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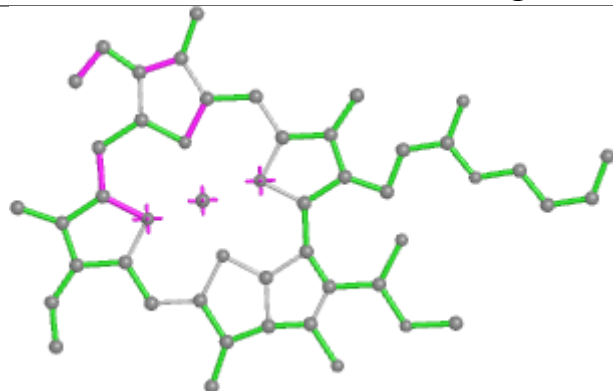
Ligand CLA A 1138



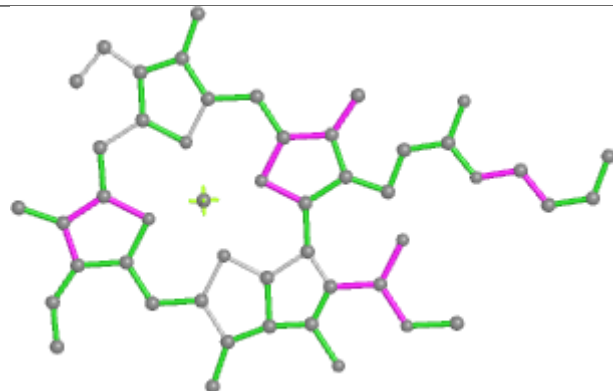
Ligand CLA A 1128



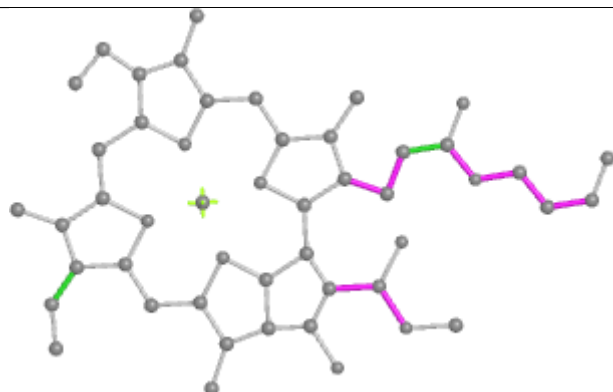
Ligand CLA J 1302



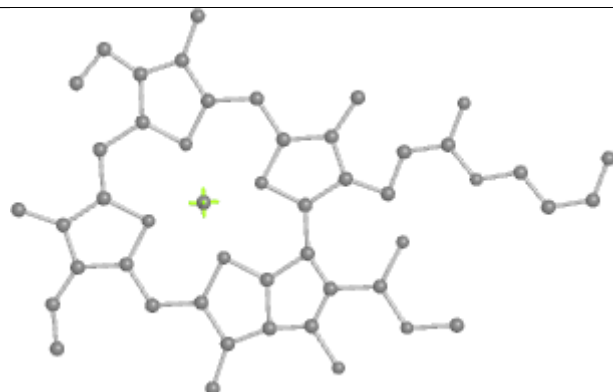
Bond lengths



Bond angles

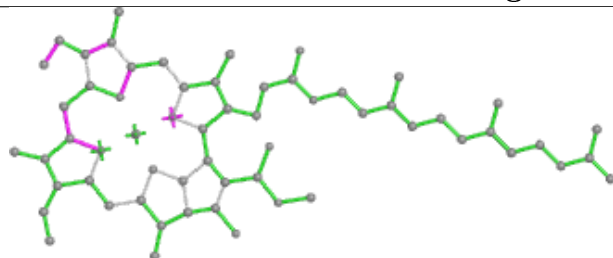


Torsions

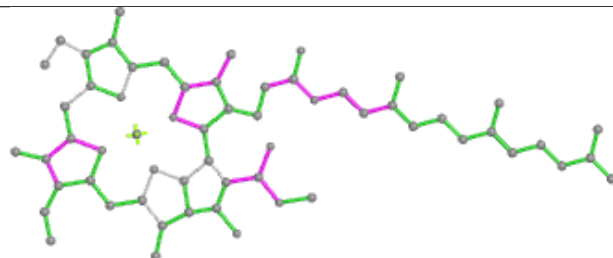


Rings

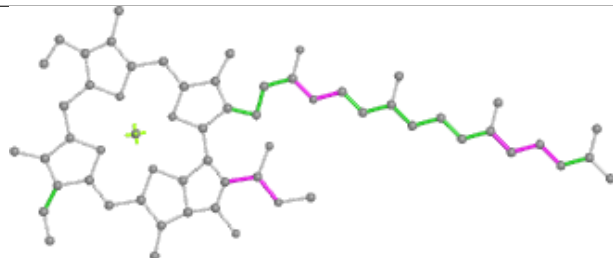
Ligand CLA B 1231



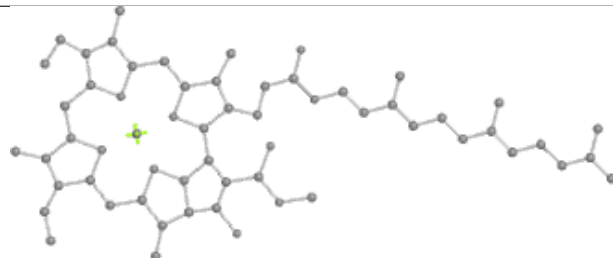
Bond lengths



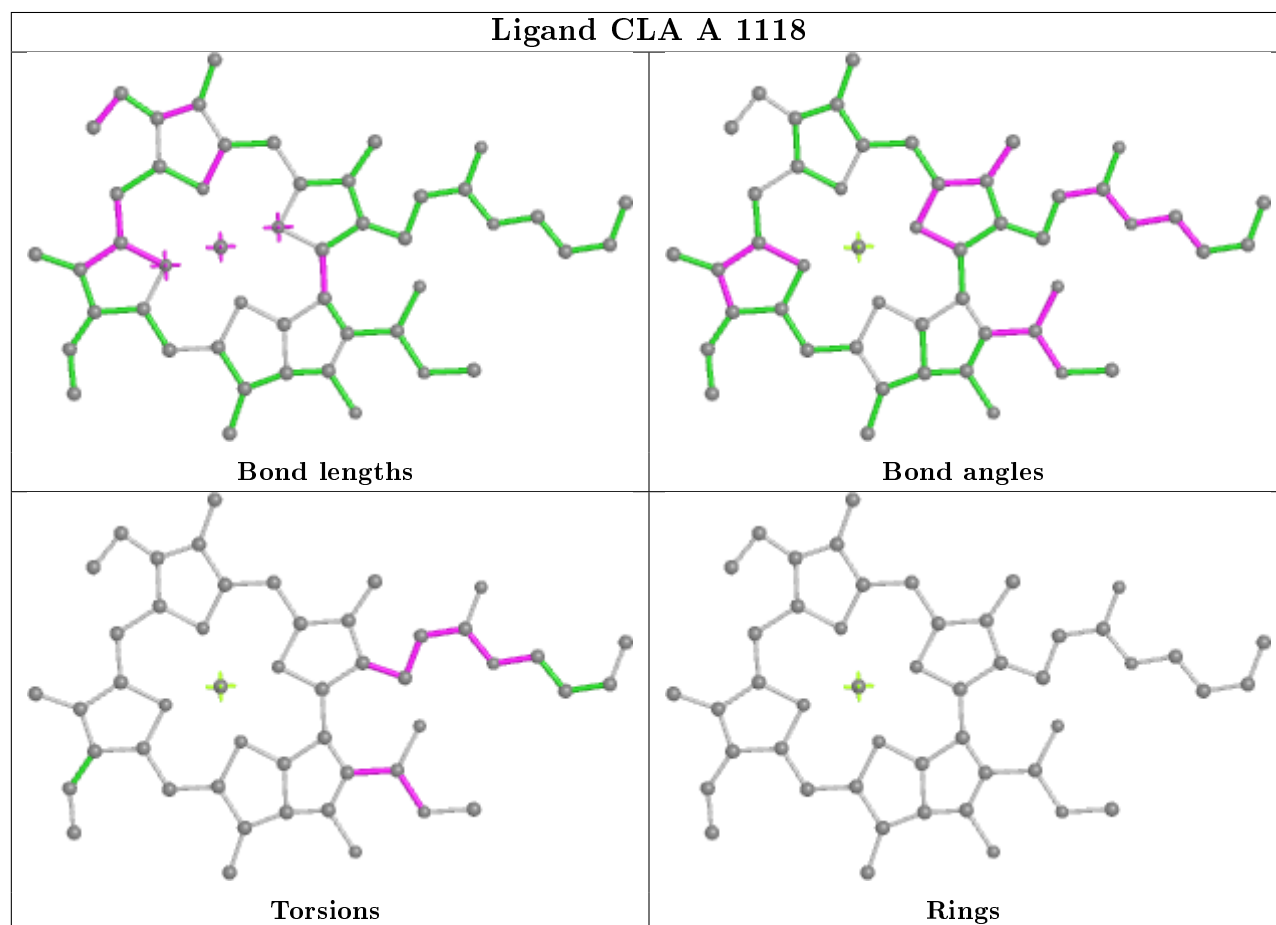
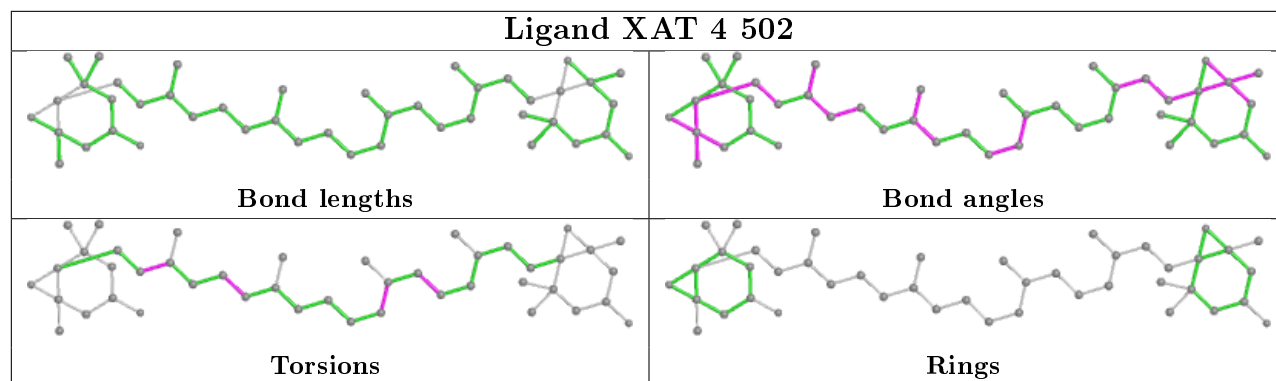
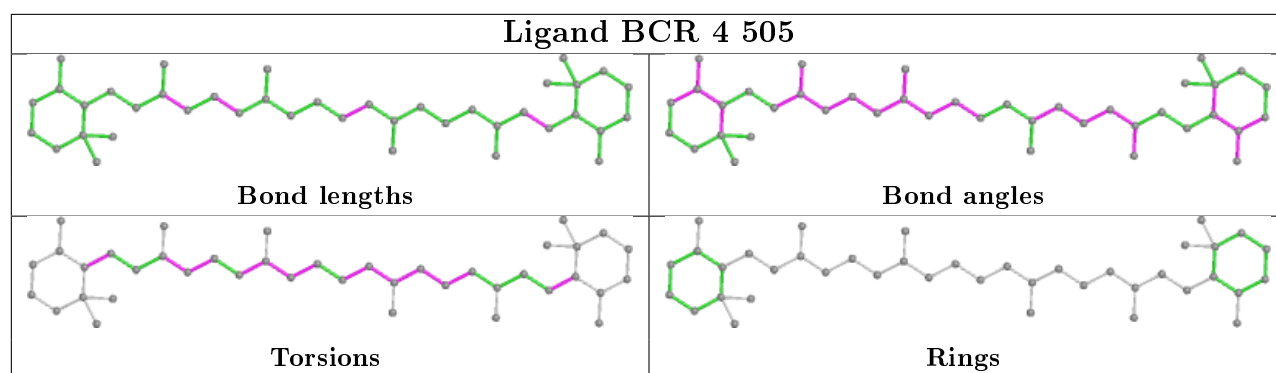
Bond angles



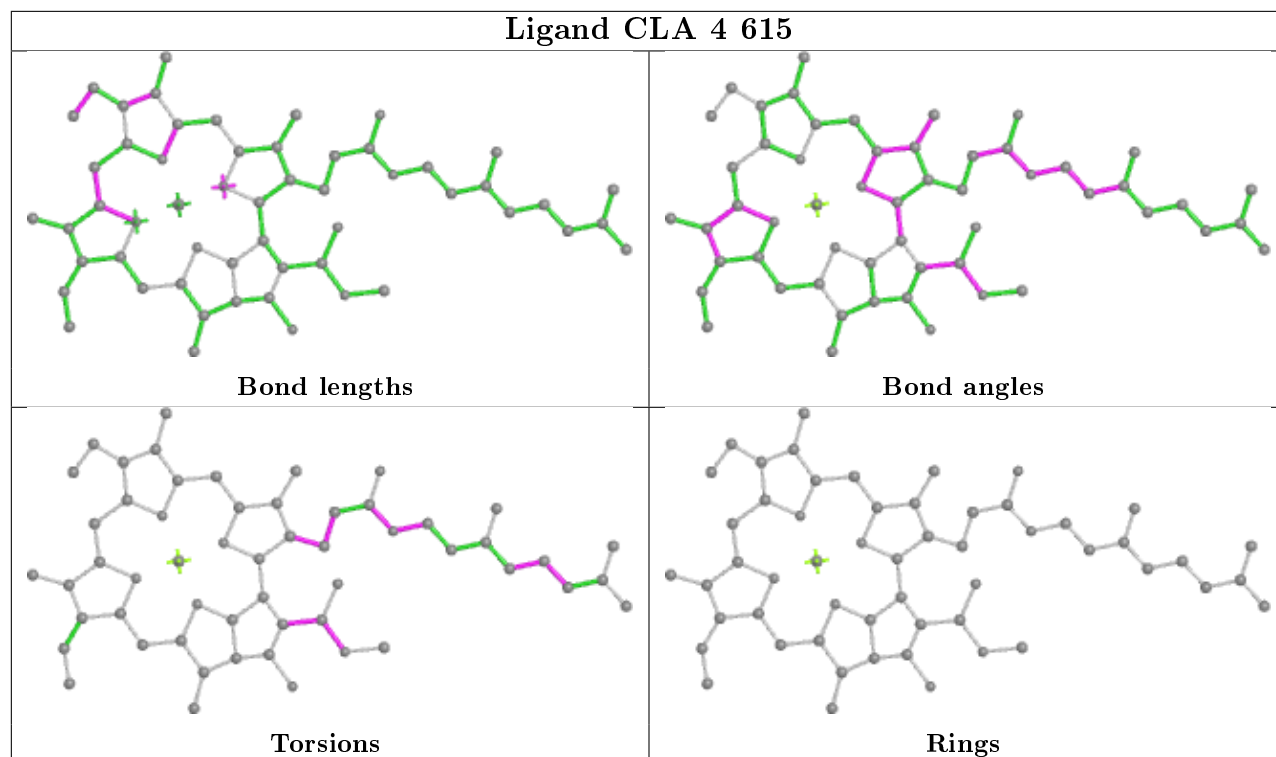
Torsions



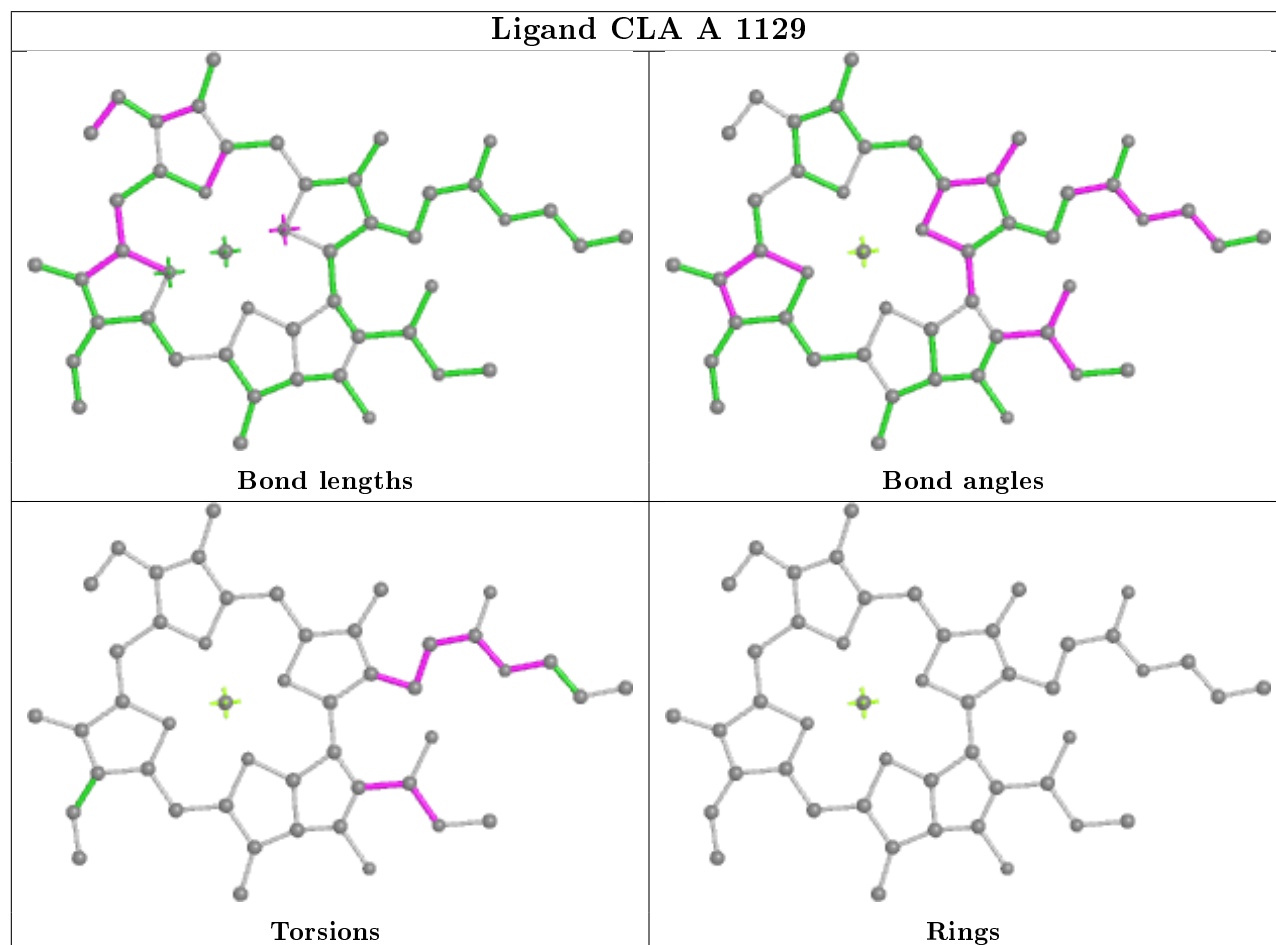
Rings

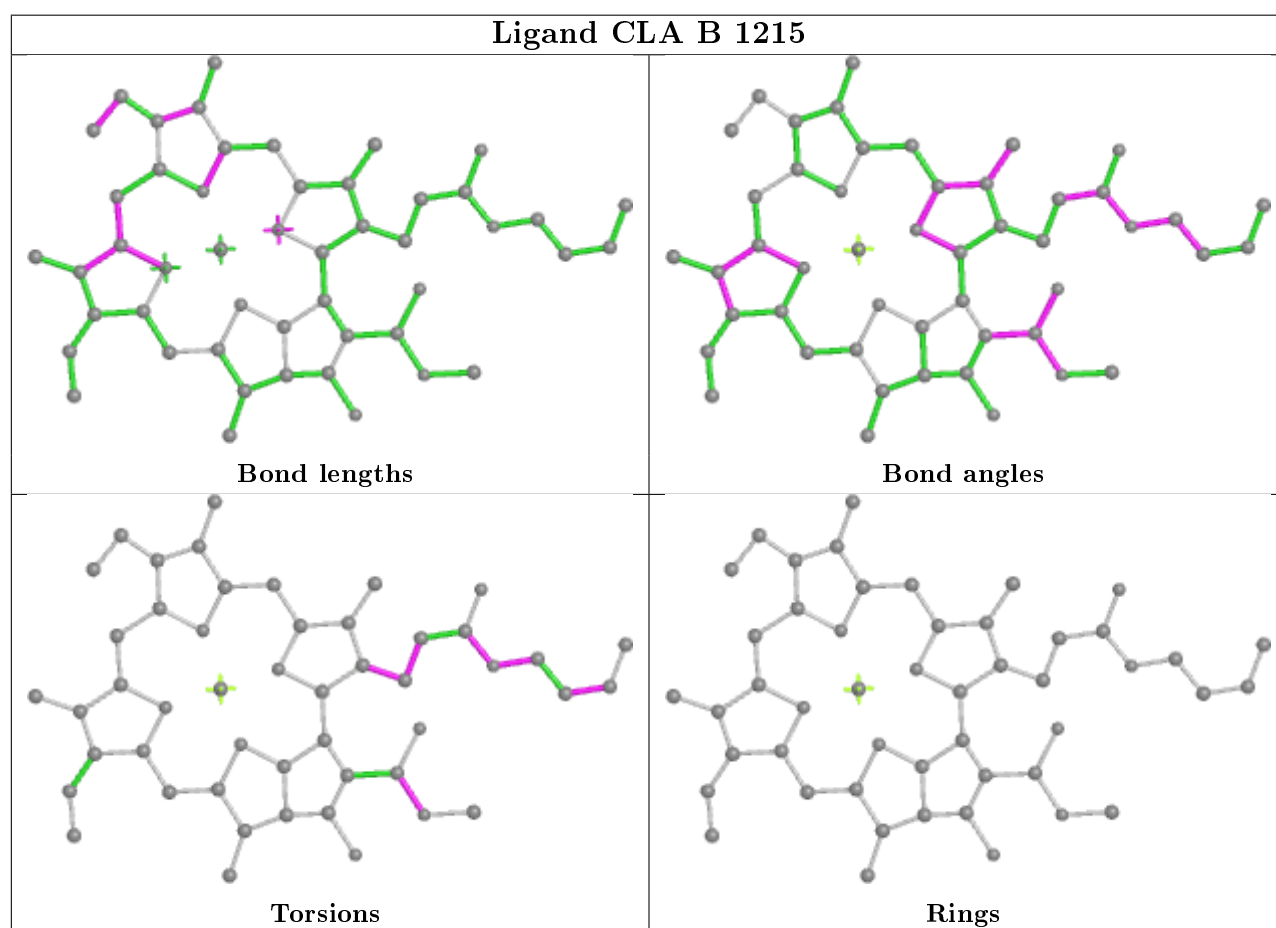
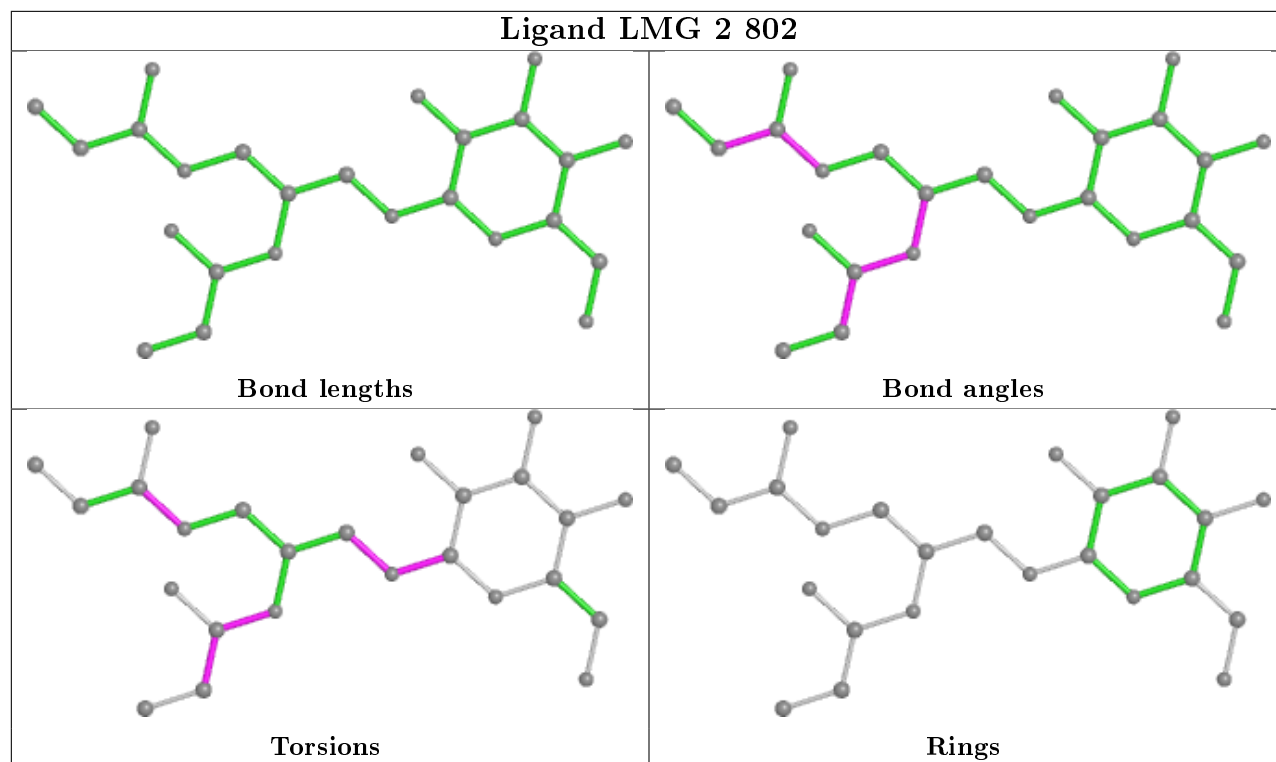


Ligand CLA 4 615

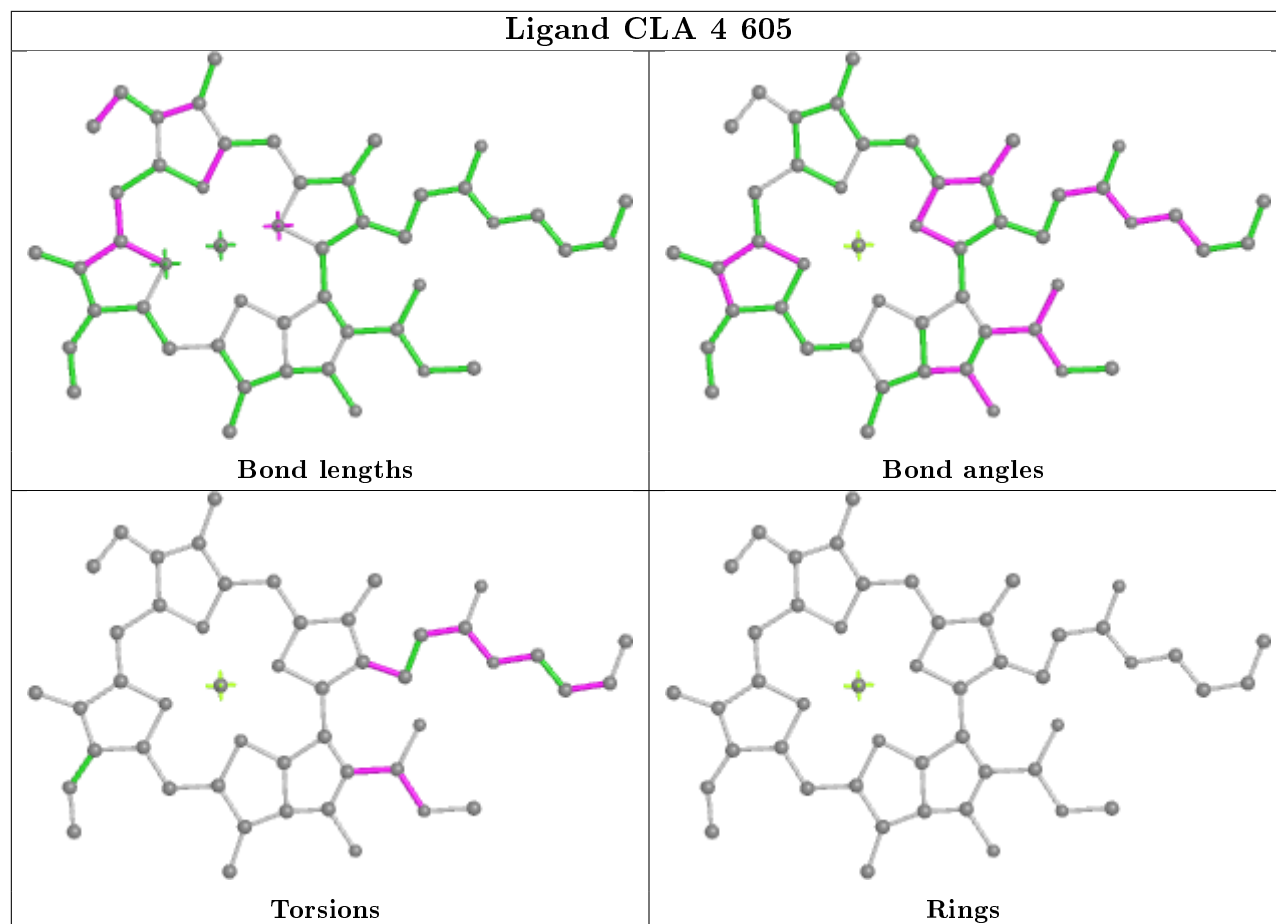


Ligand CLA A 1129

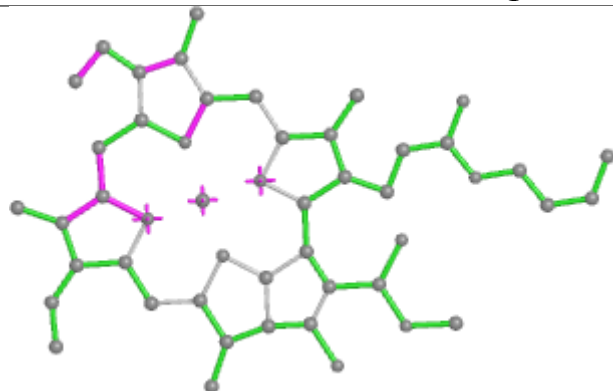




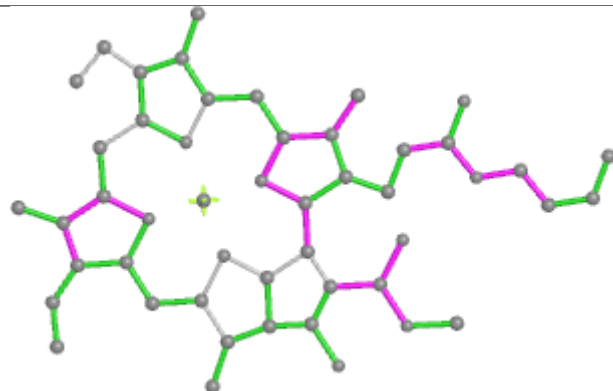
Ligand CLA 4 605



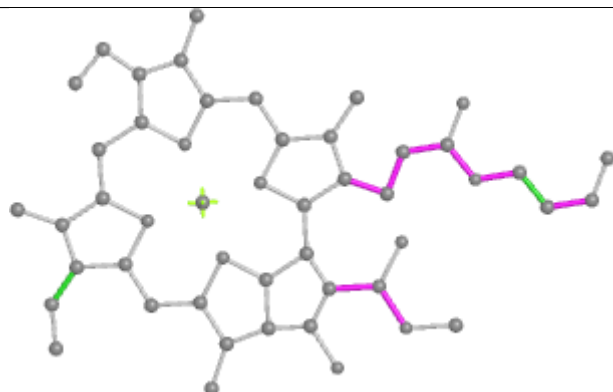
Ligand CLA B 1224



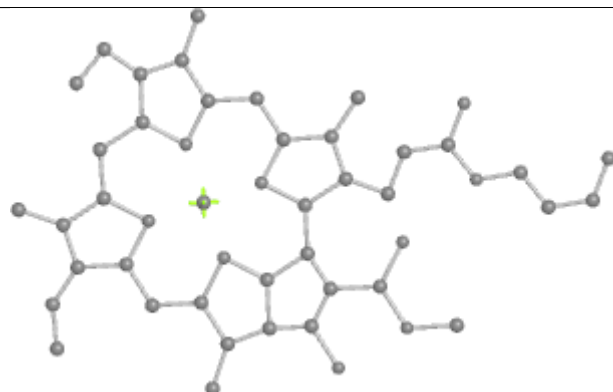
Bond lengths



Bond angles

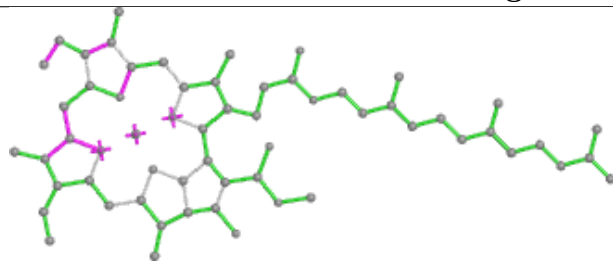


Torsions

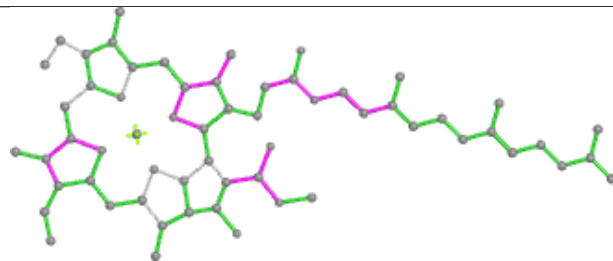


Rings

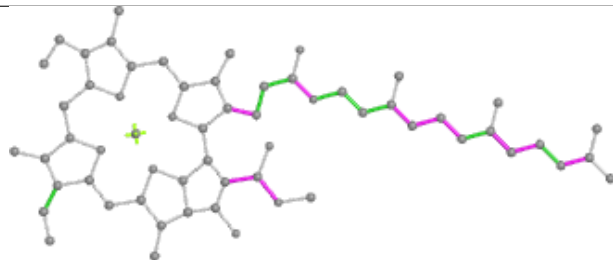
Ligand CLA A 1104



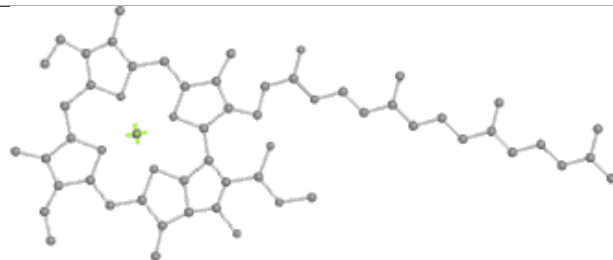
Bond lengths



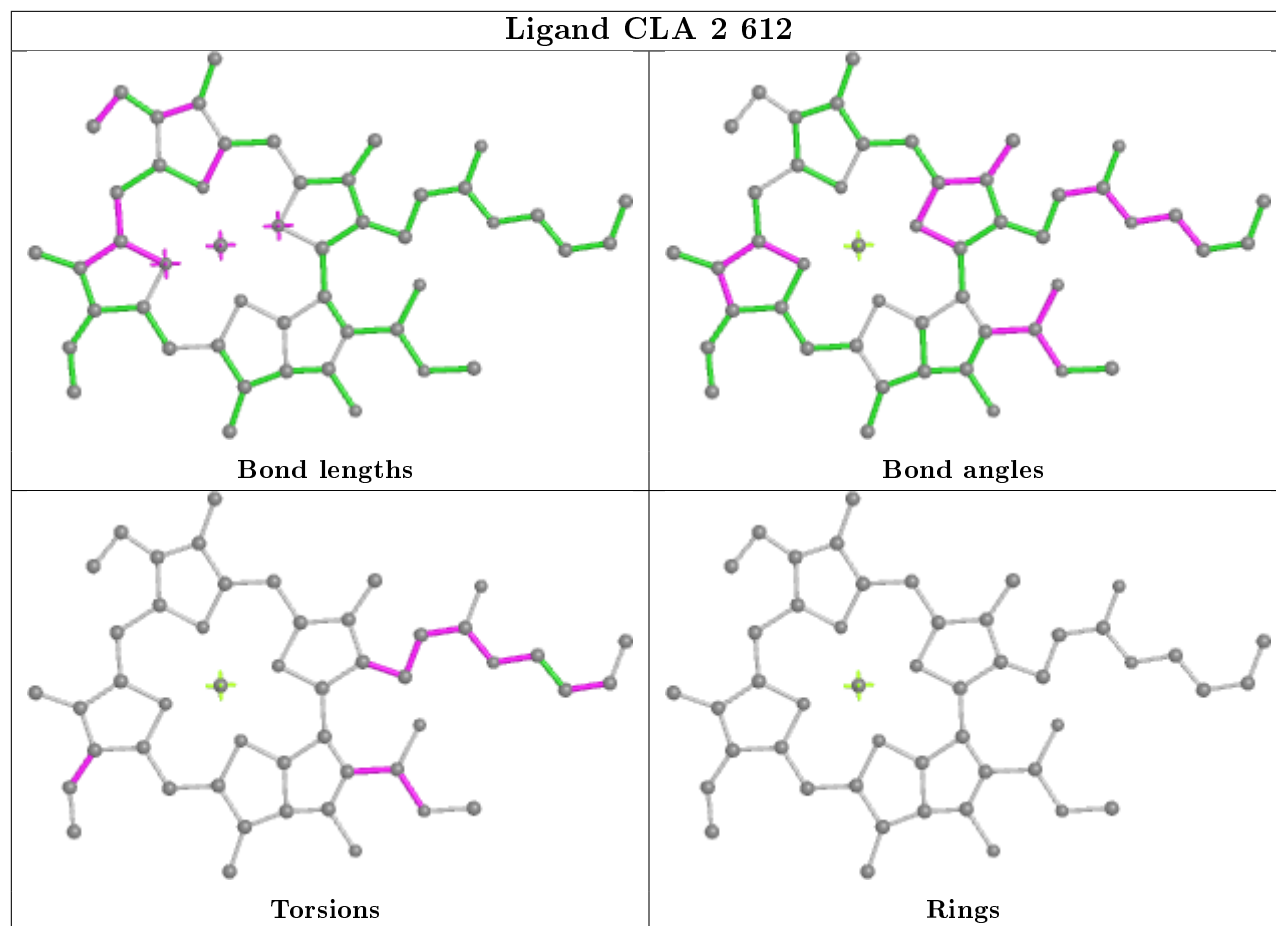
Bond angles

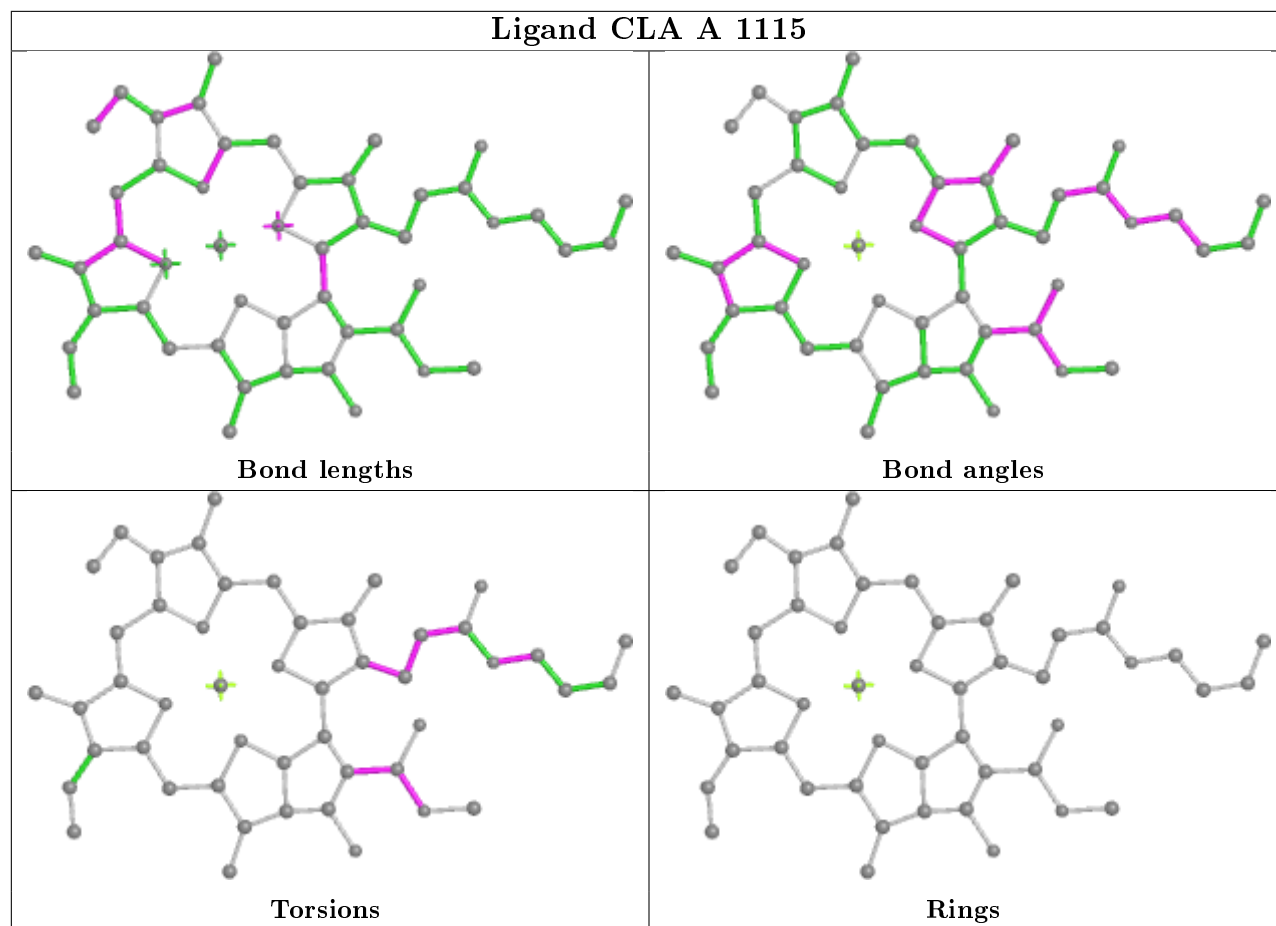


Torsions

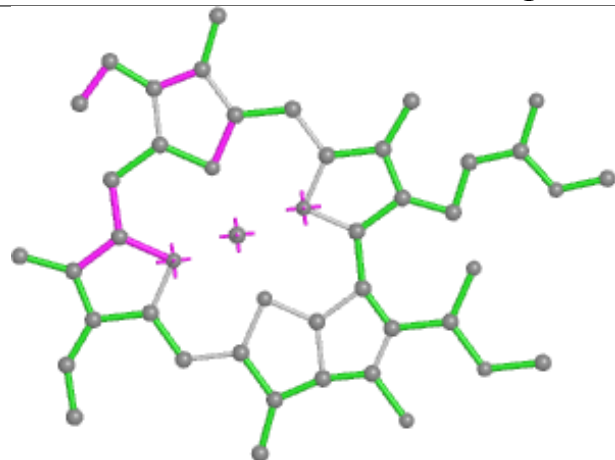


Rings

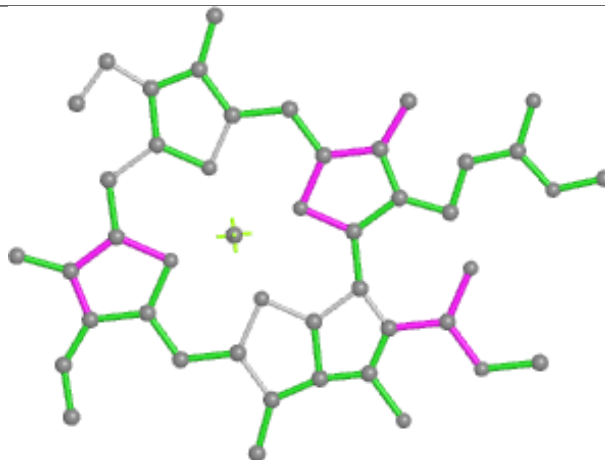




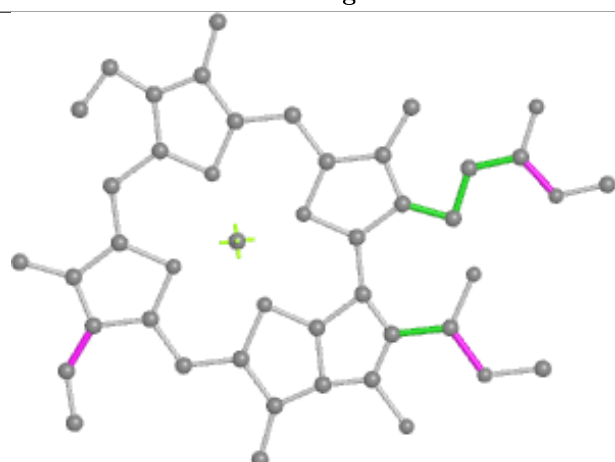
Ligand CLA 3 605



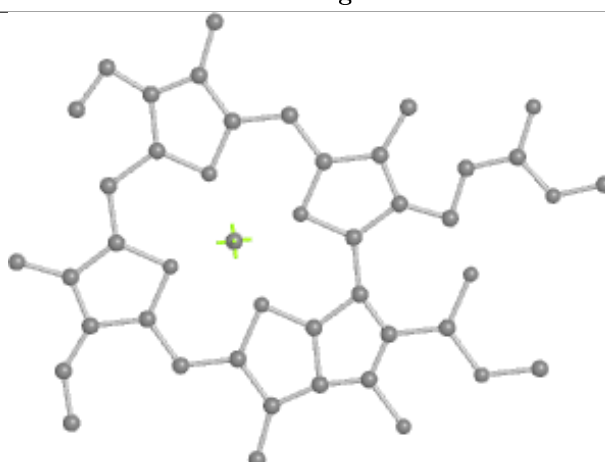
Bond lengths



Bond angles

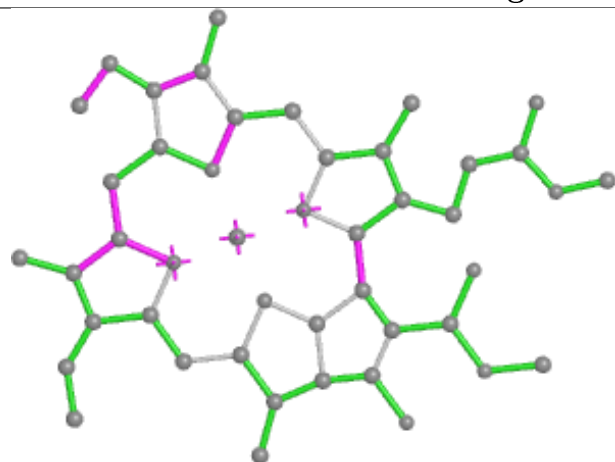


Torsions

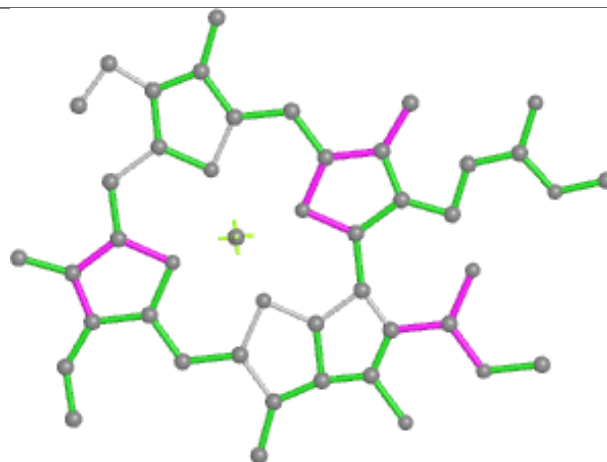


Rings

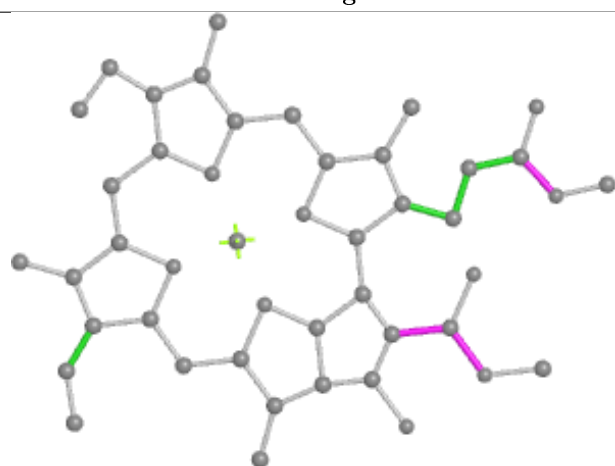
Ligand CLA A 1114



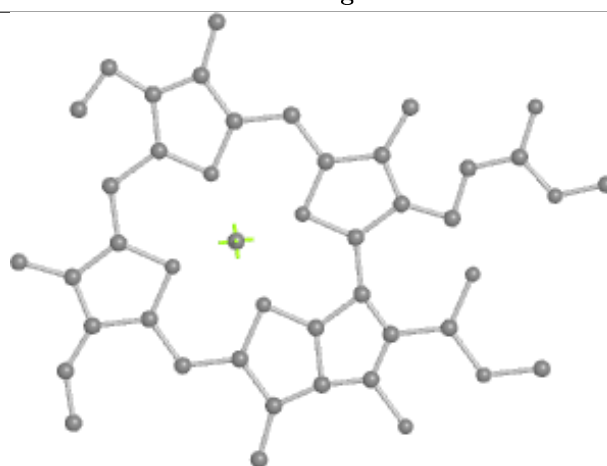
Bond lengths



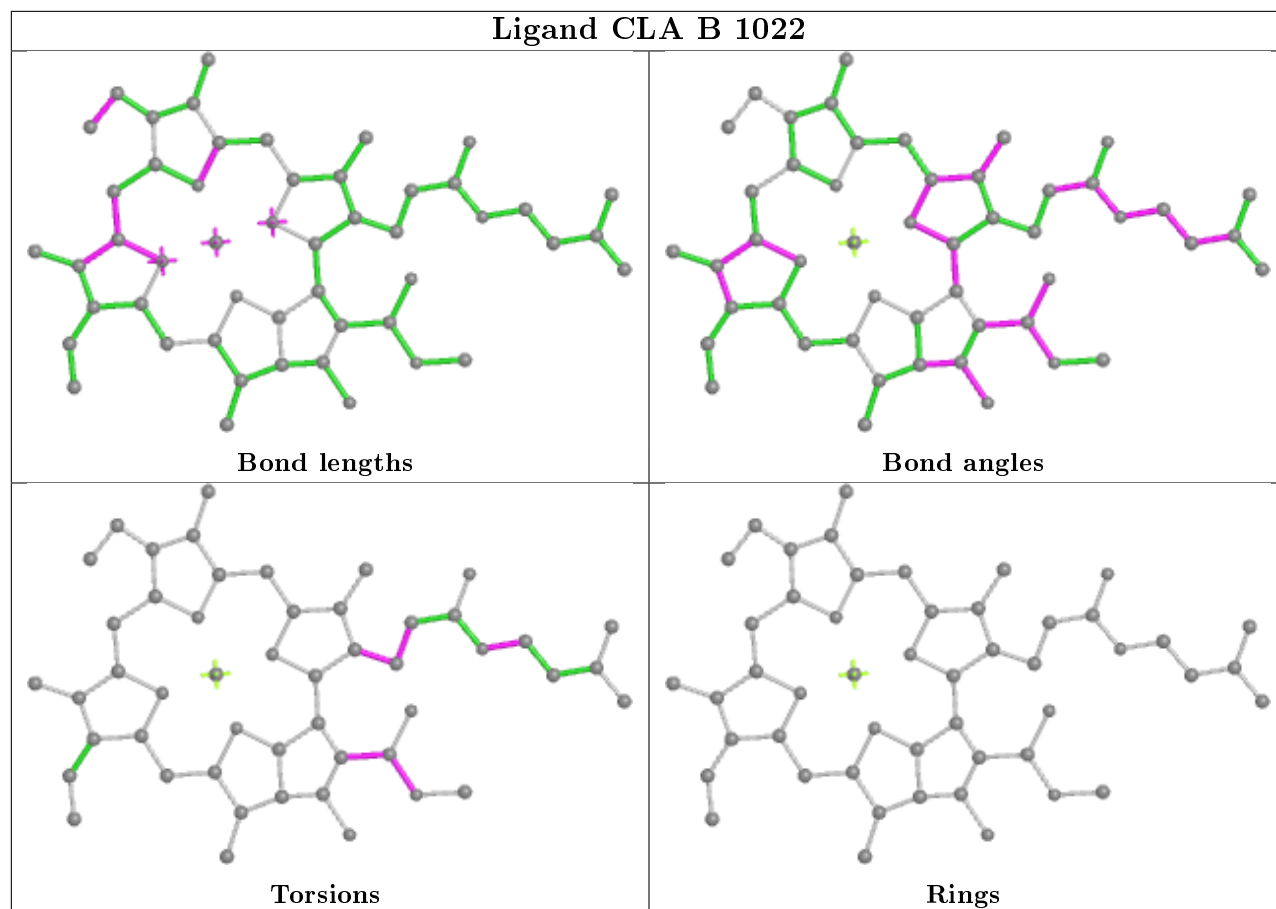
Bond angles



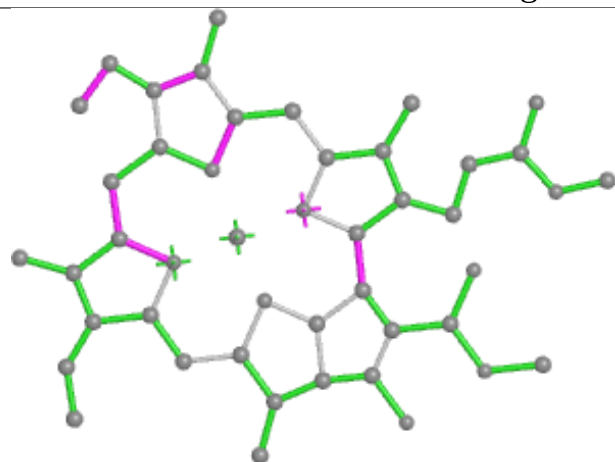
Torsions



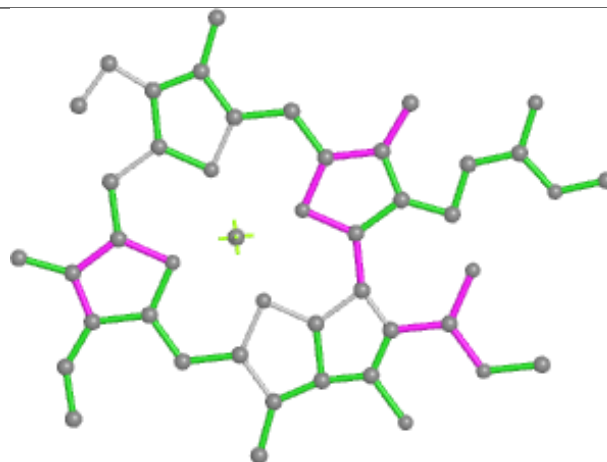
Rings



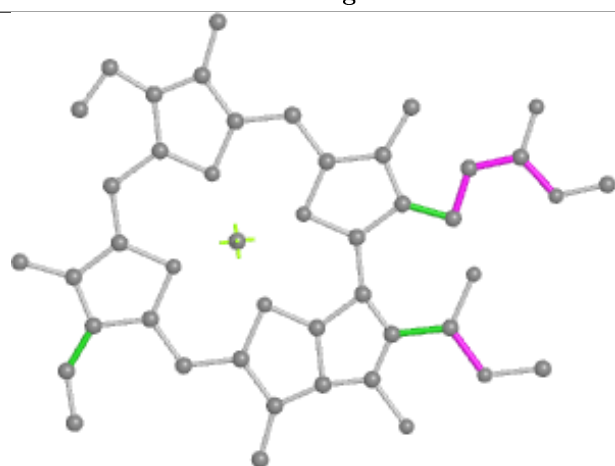
Ligand CLA 3 615



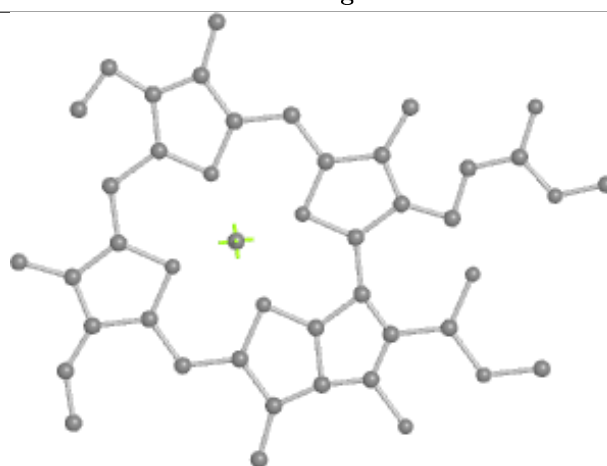
Bond lengths



Bond angles

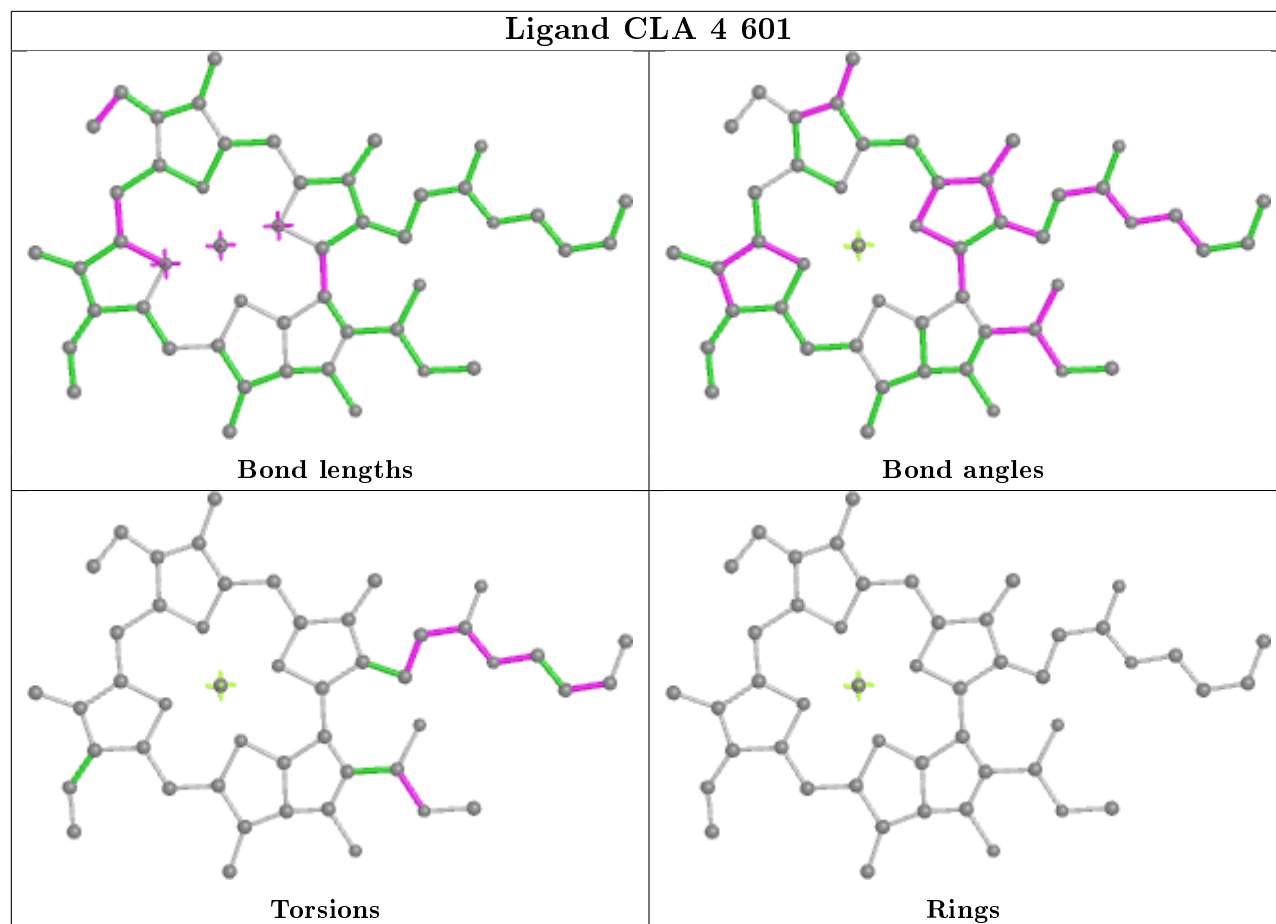


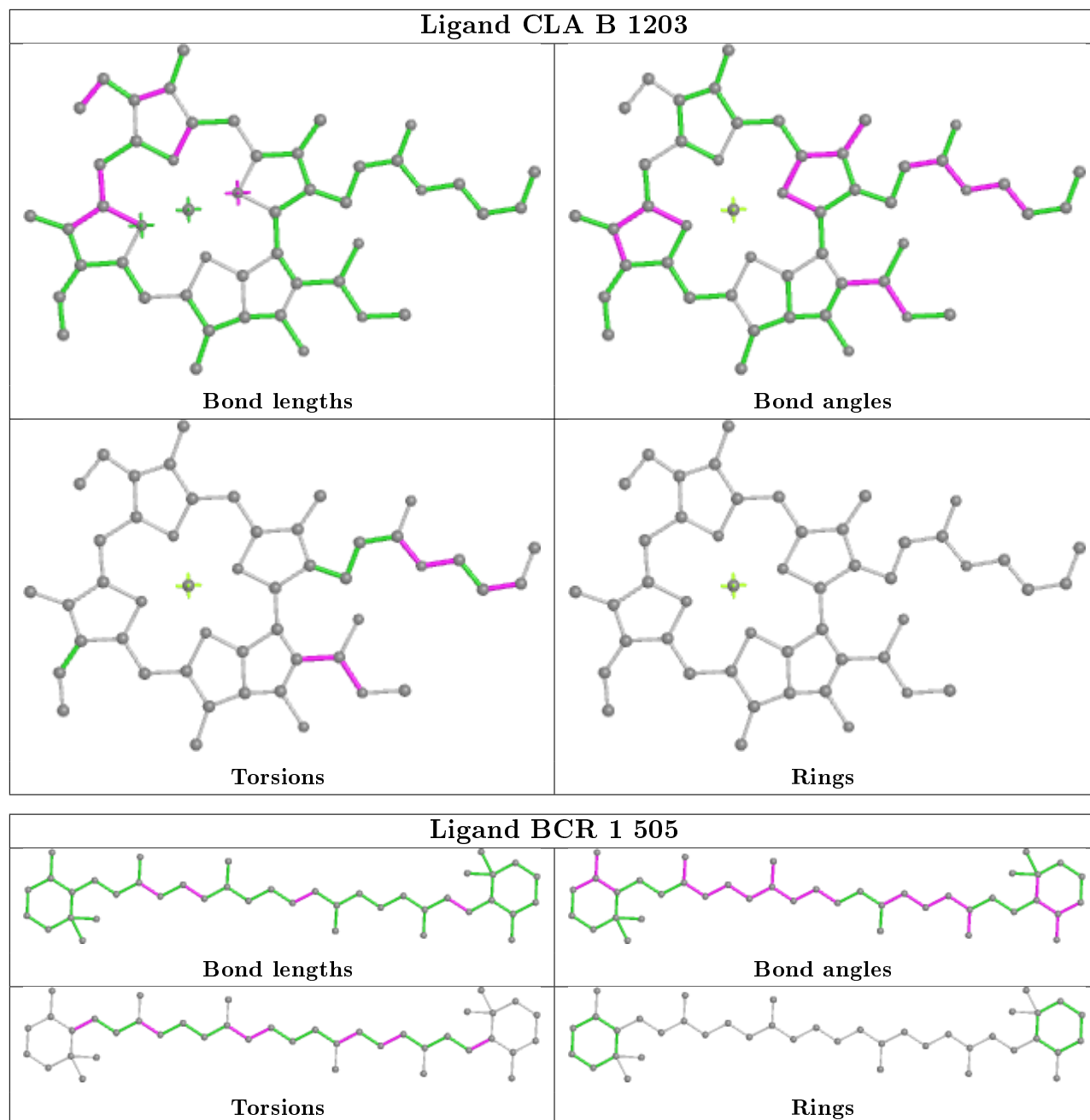
Torsions



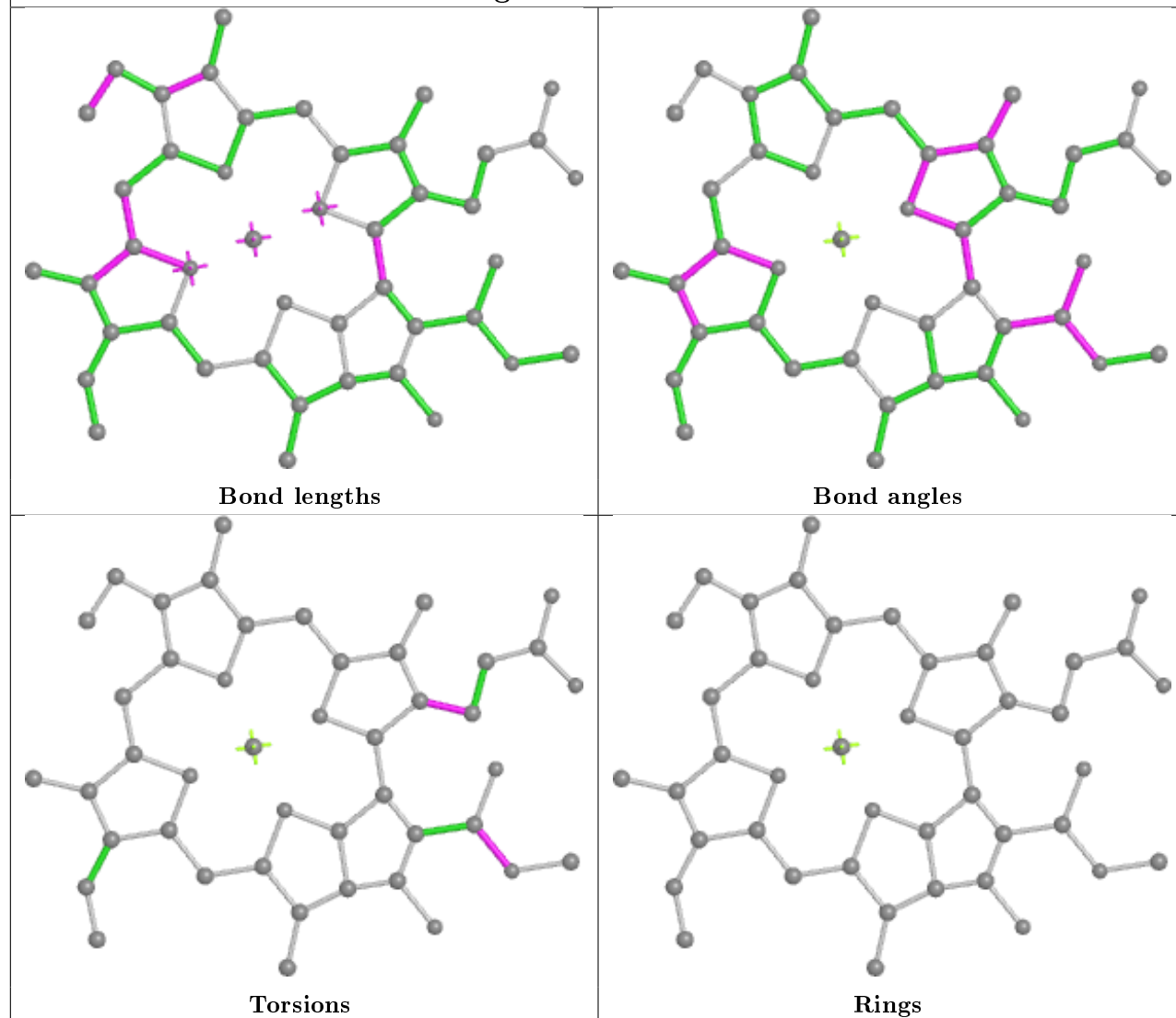
Rings

Ligand CLA 4 601

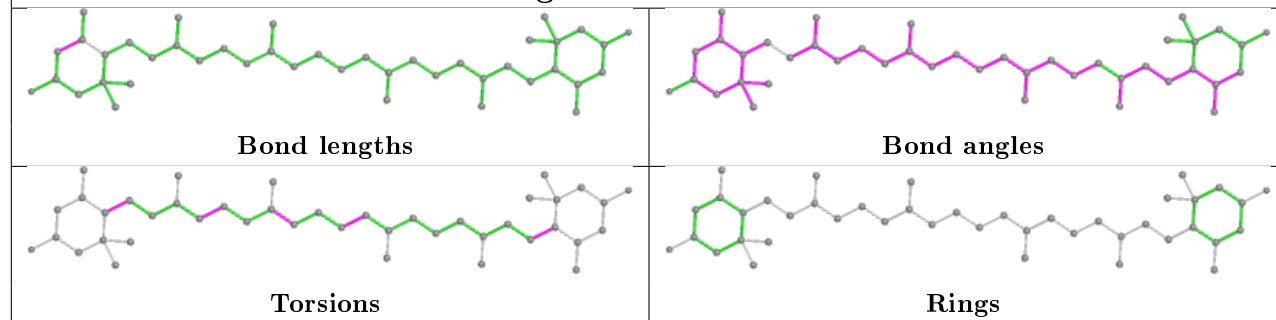




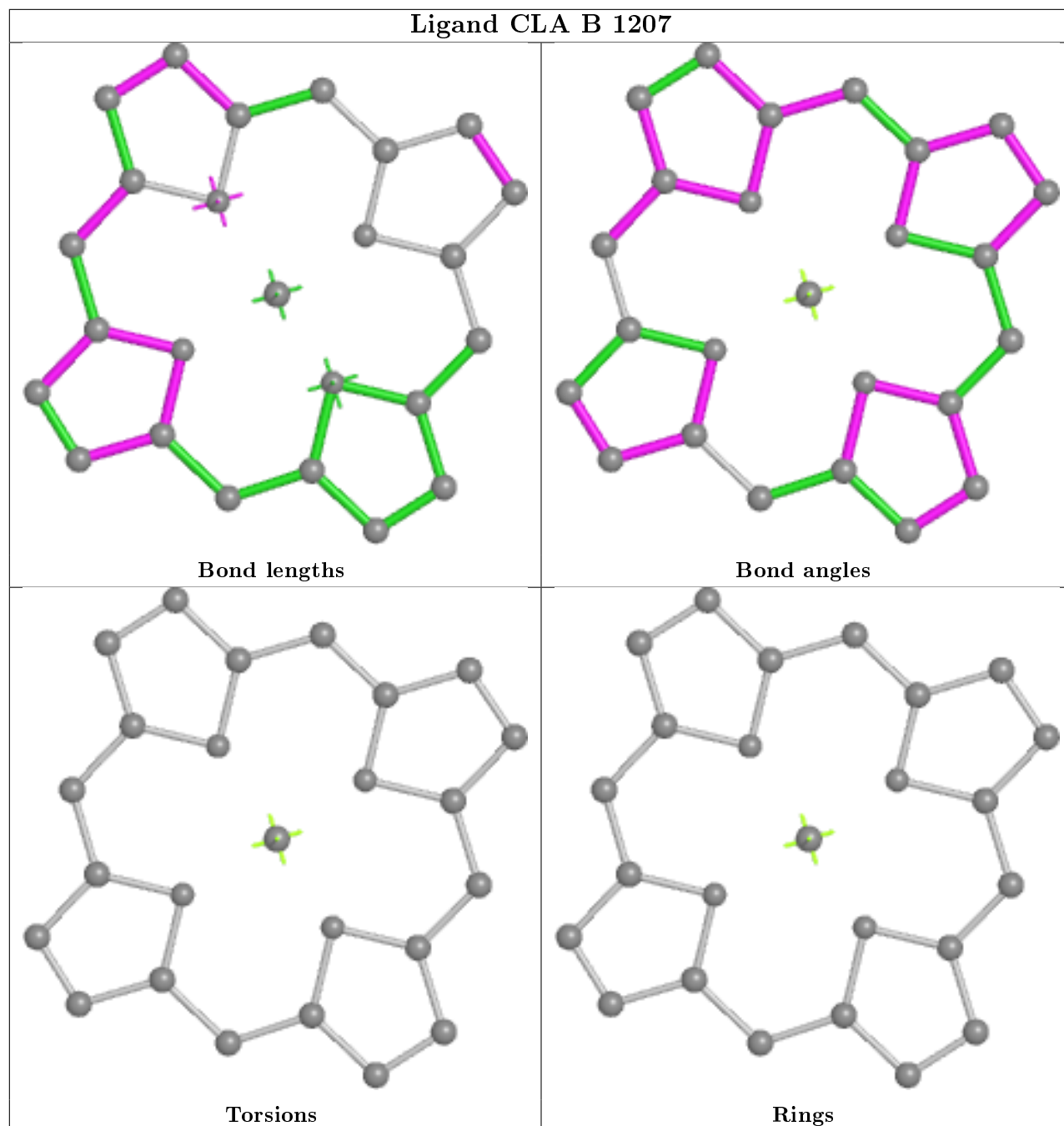
Ligand CLA 1 613



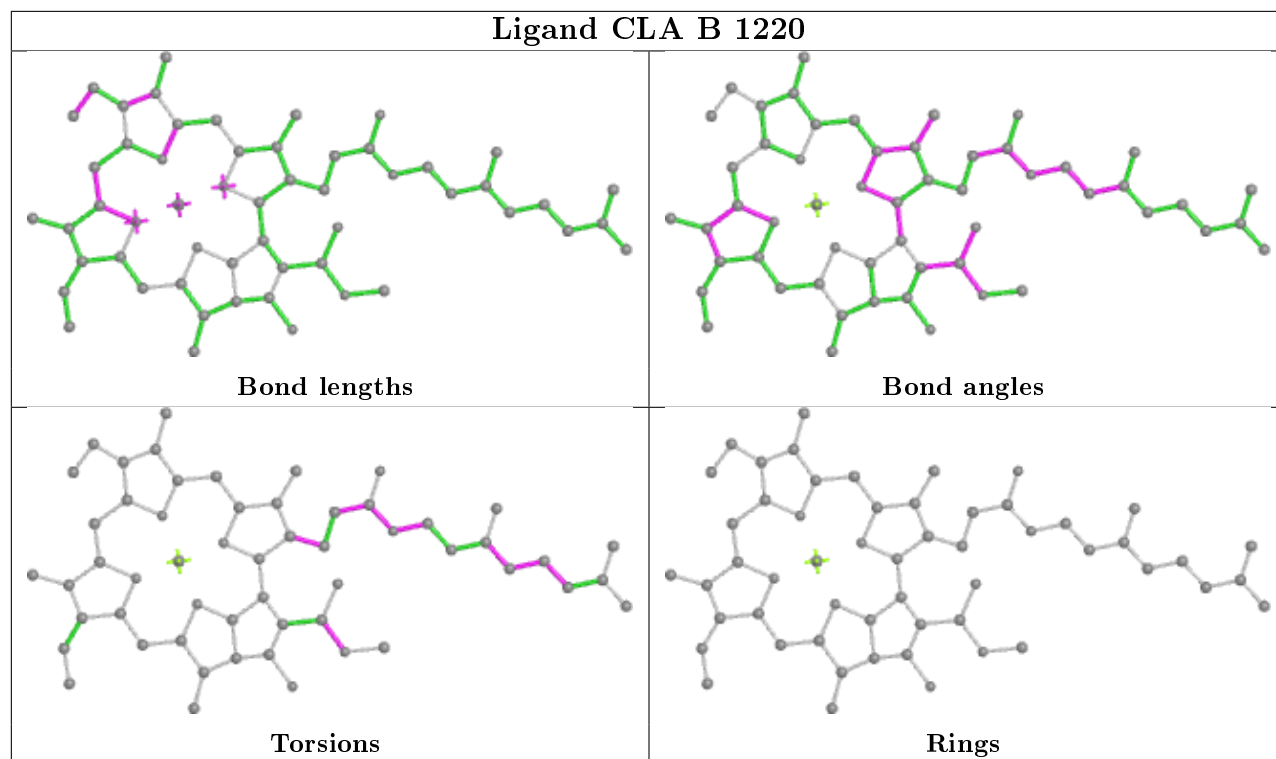
Ligand LUT 1 501



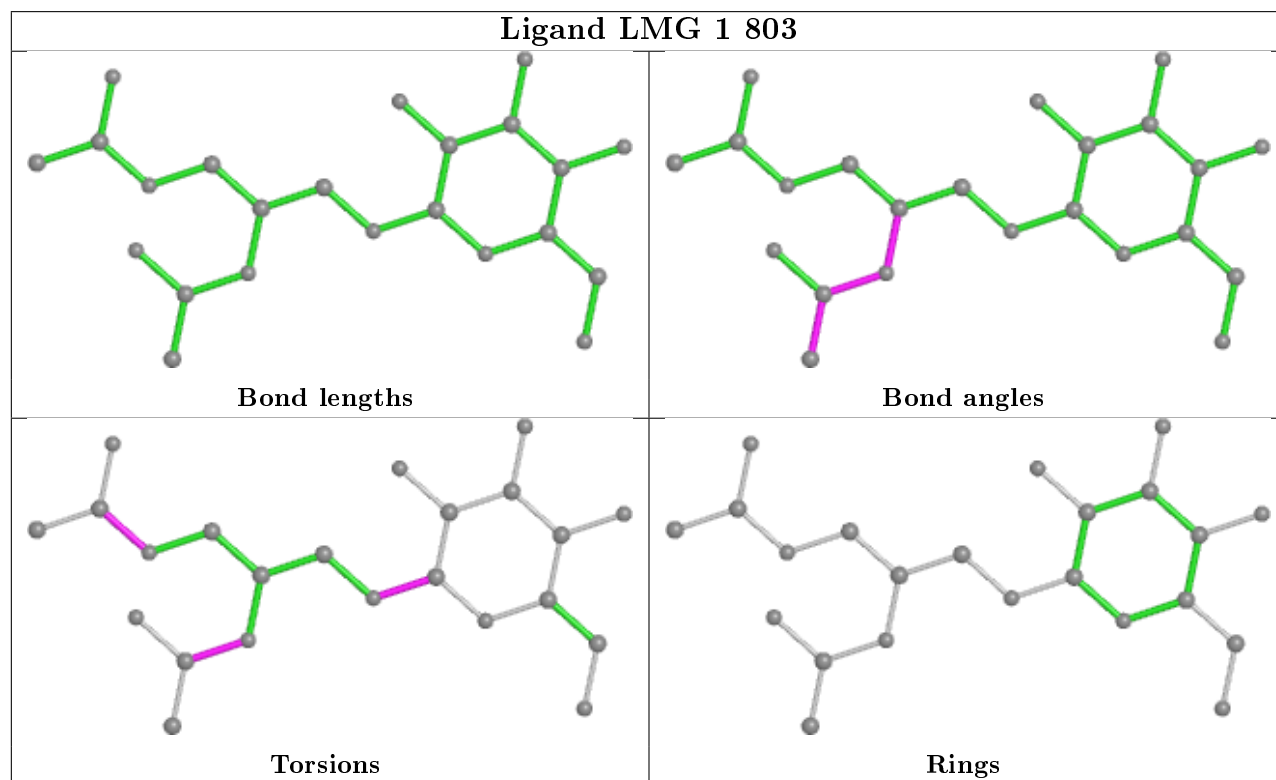
Ligand CLA B 1207



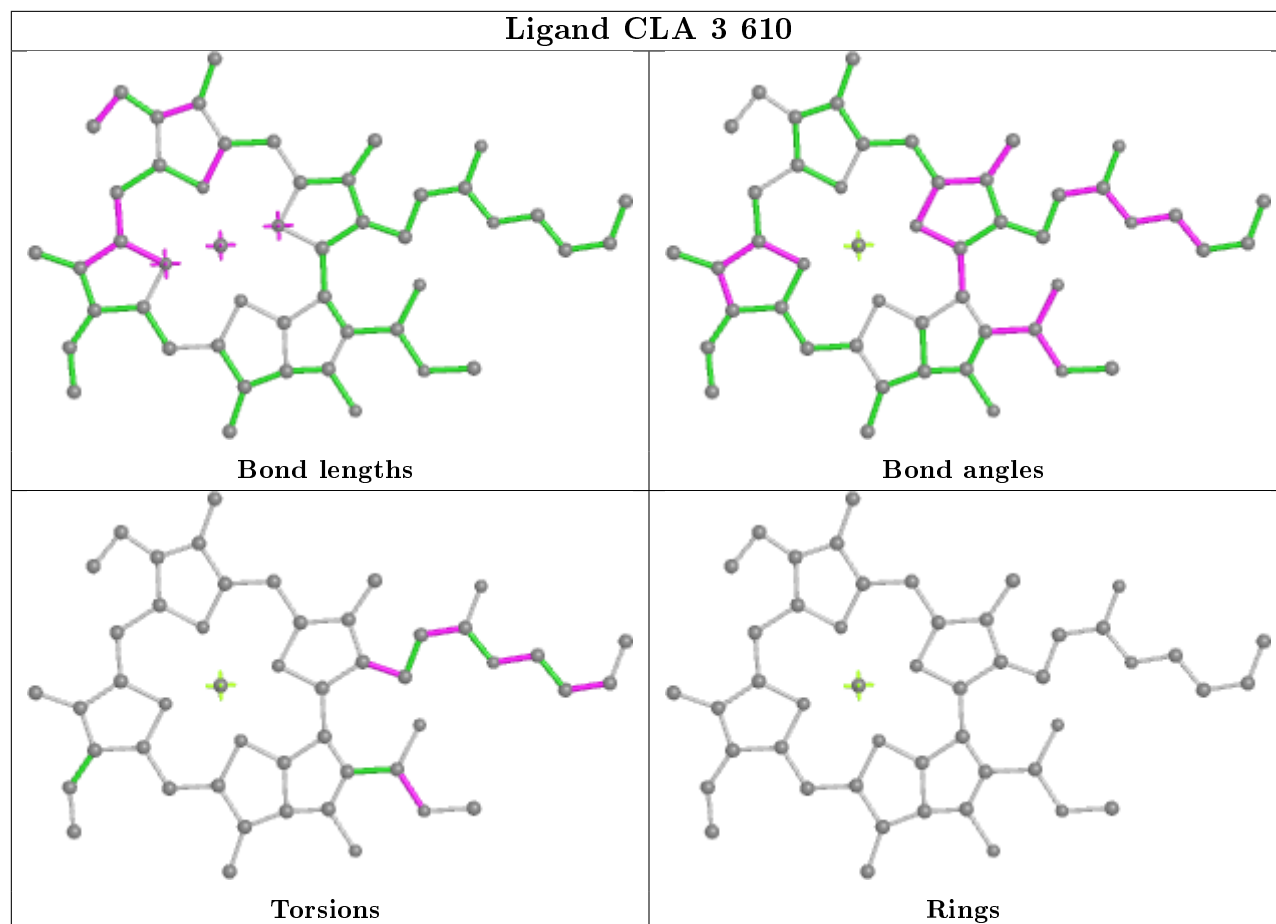
Ligand CLA B 1220

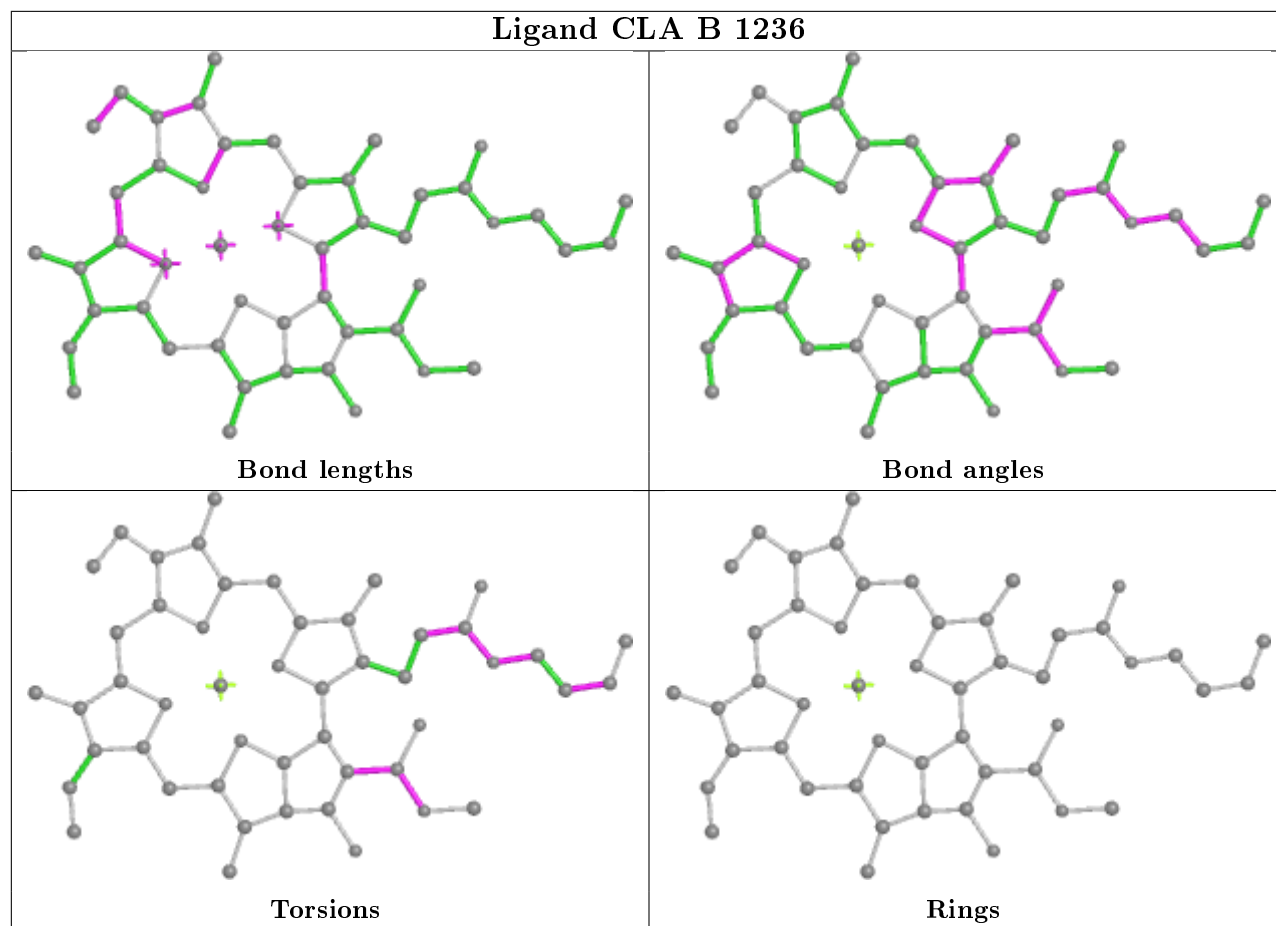


Ligand LMG 1 803

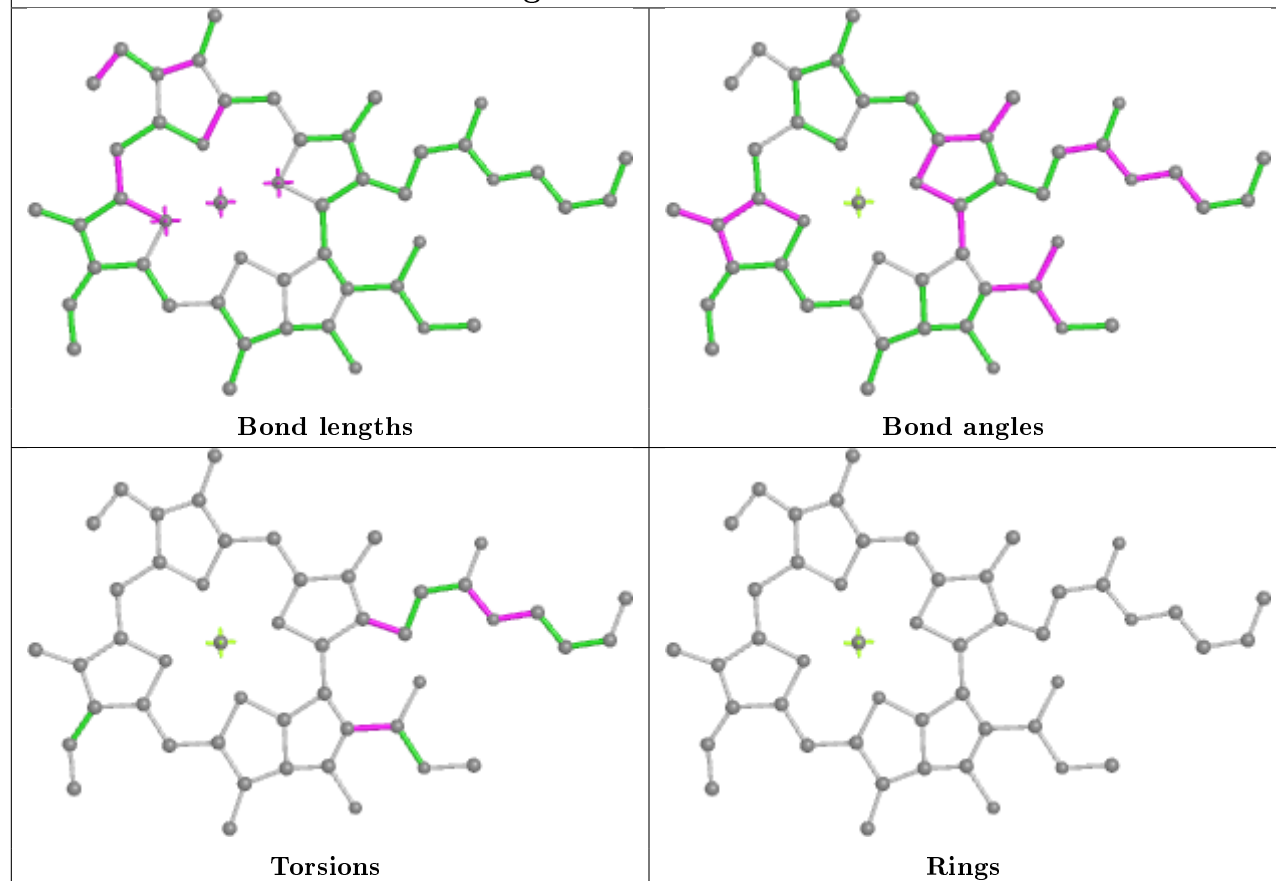


Ligand CLA 3 610

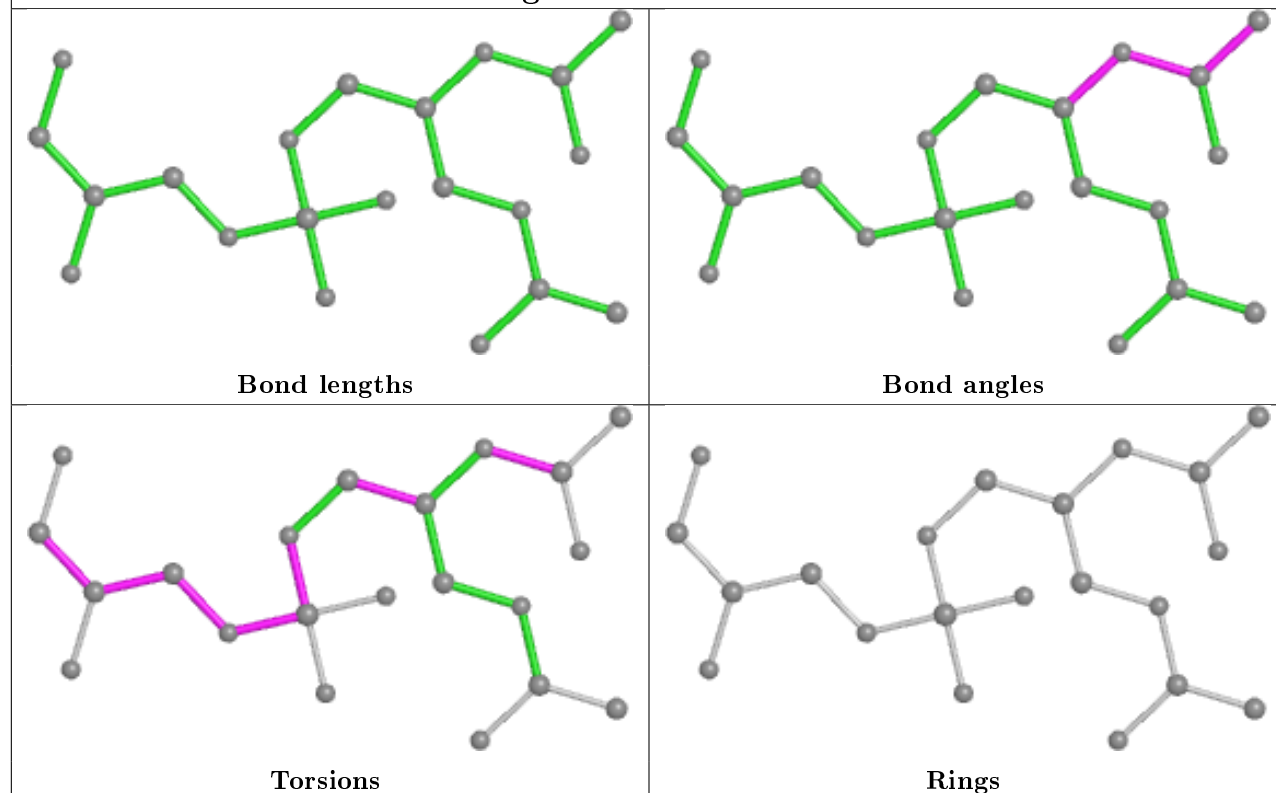




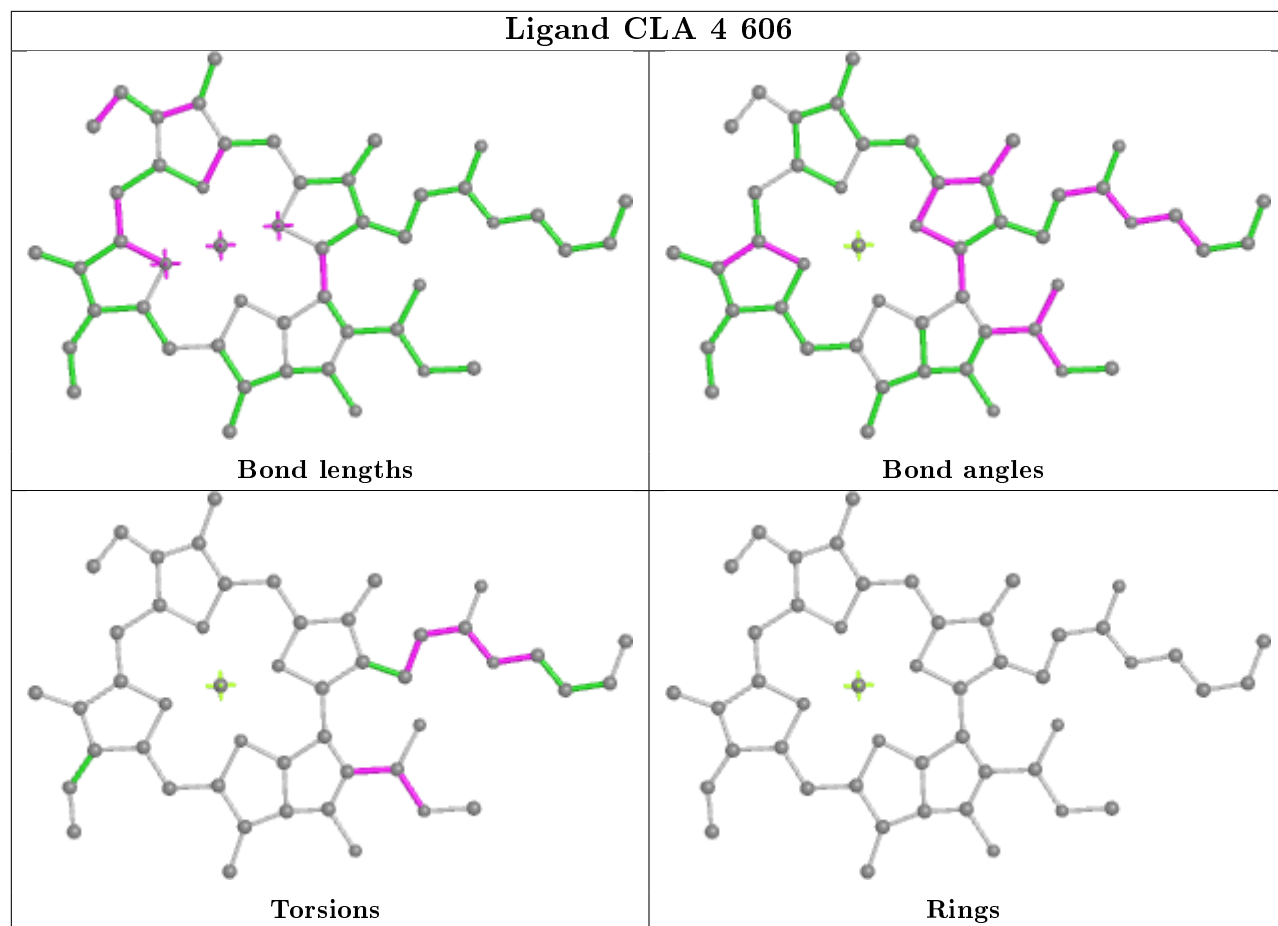
Ligand CLA A 1111

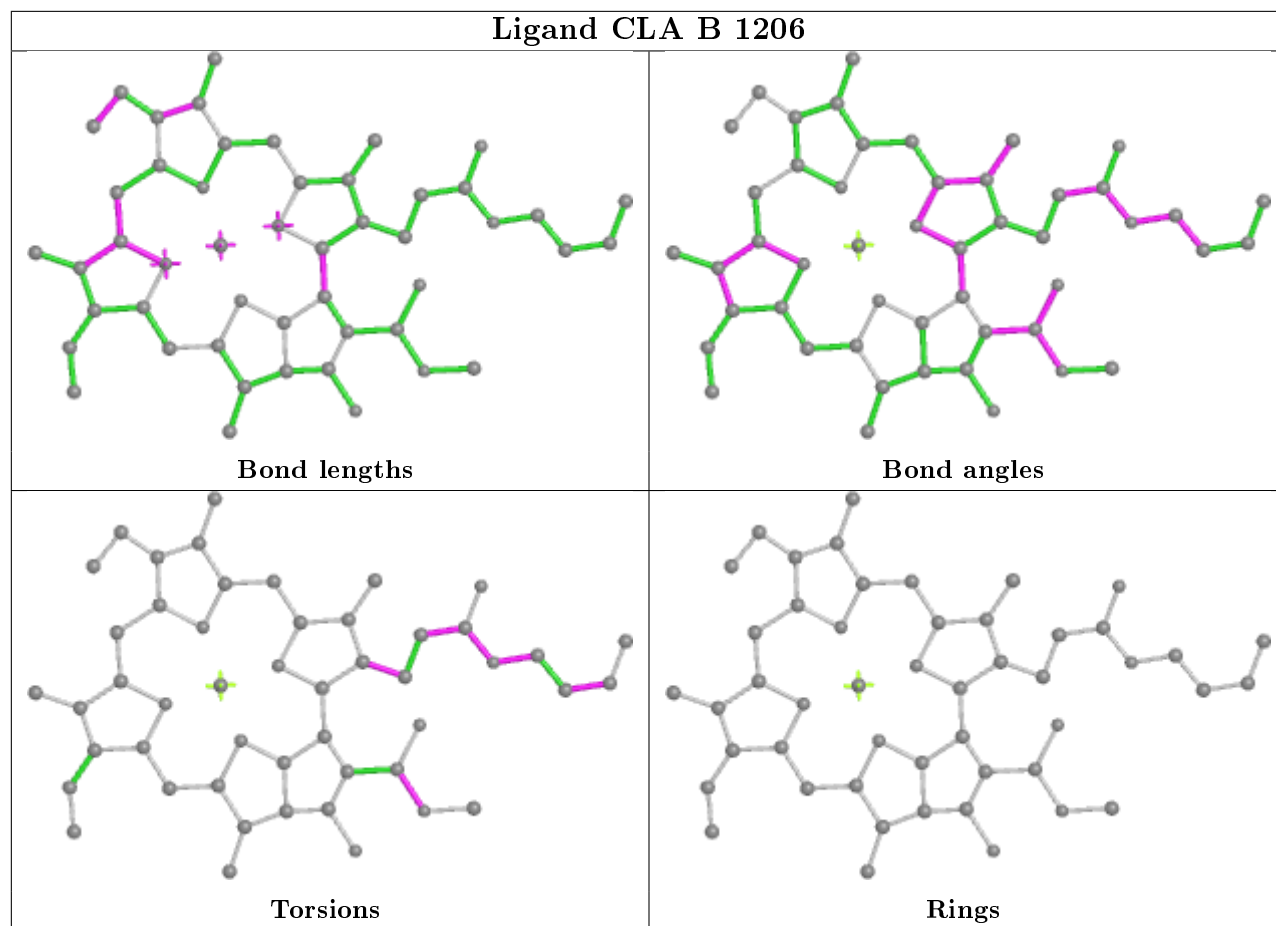


Ligand LHG B 5001

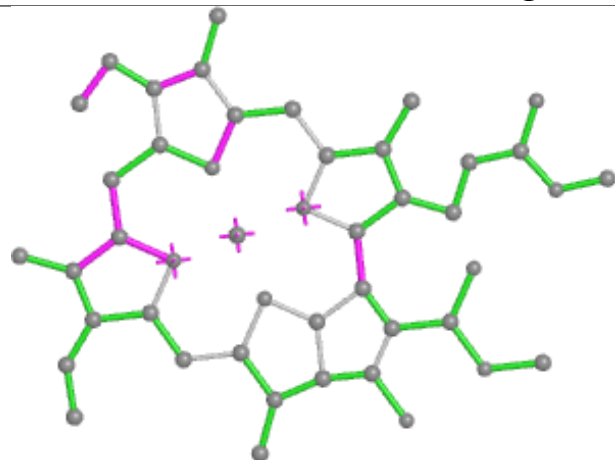


Ligand CLA 4 606

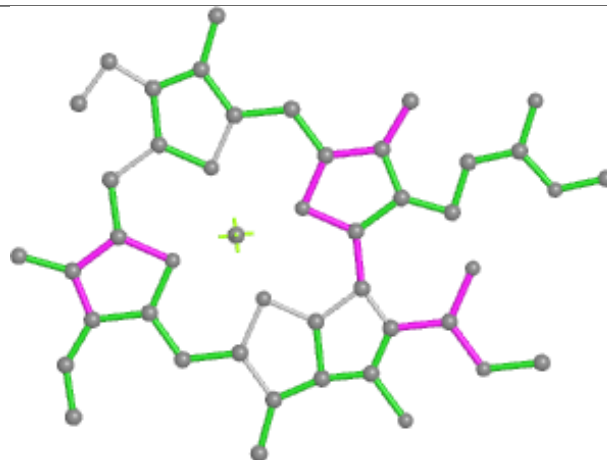




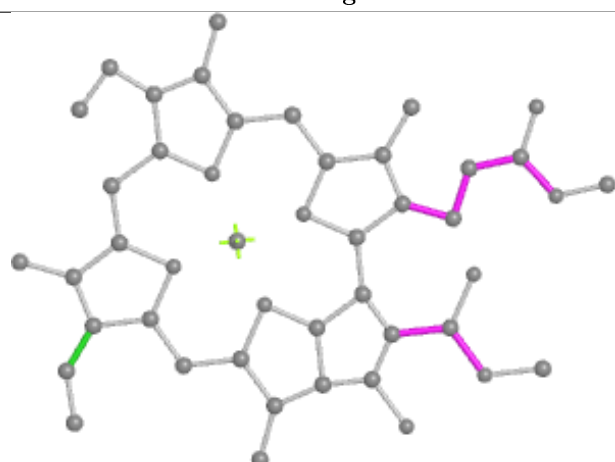
Ligand CLA 1 602



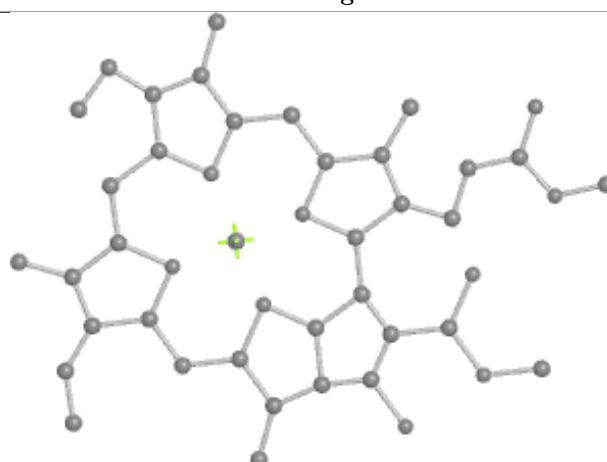
Bond lengths



Bond angles

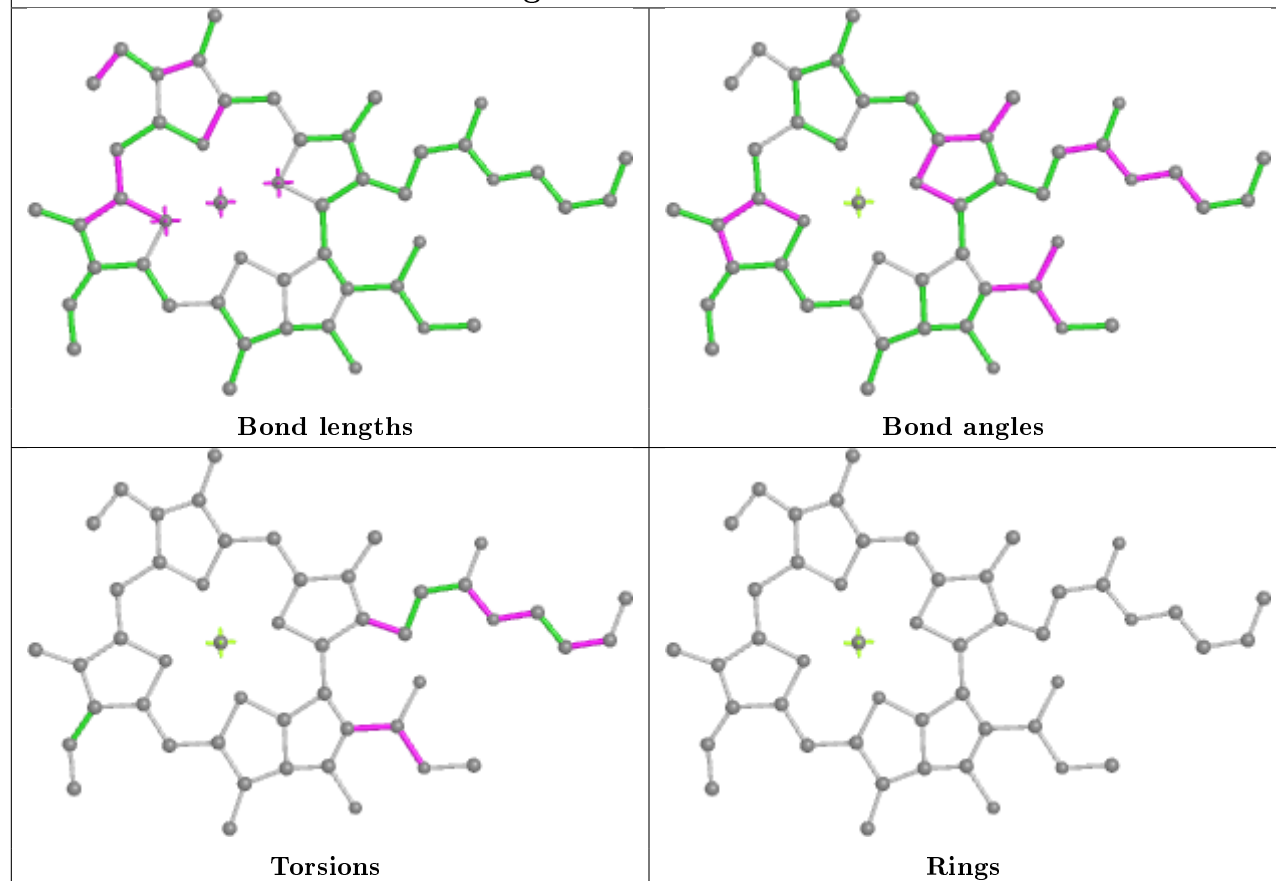


Torsions

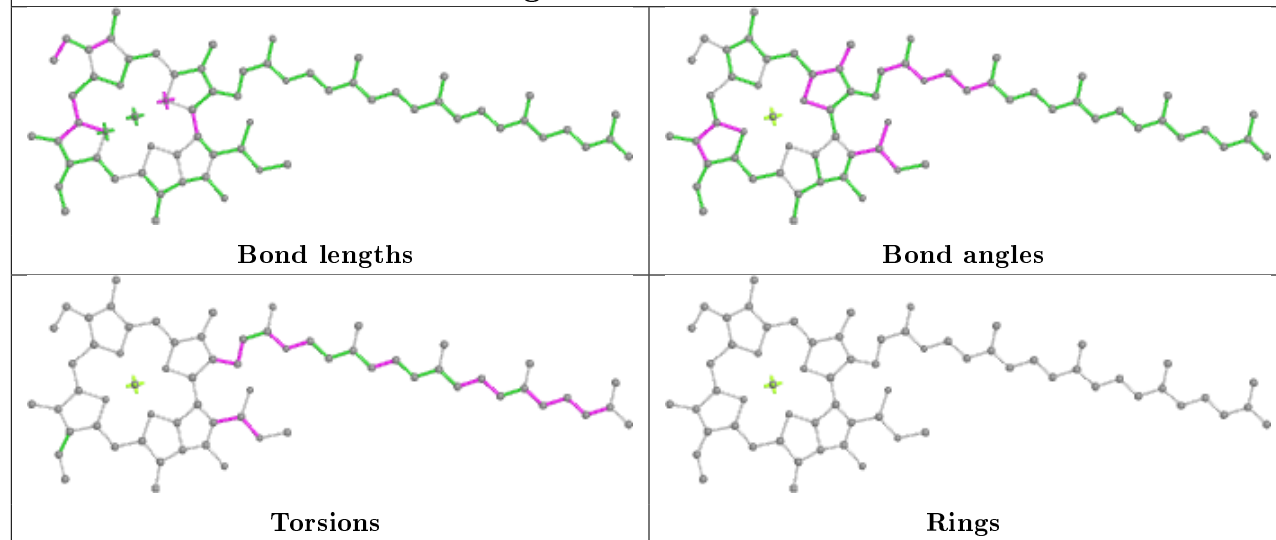


Rings

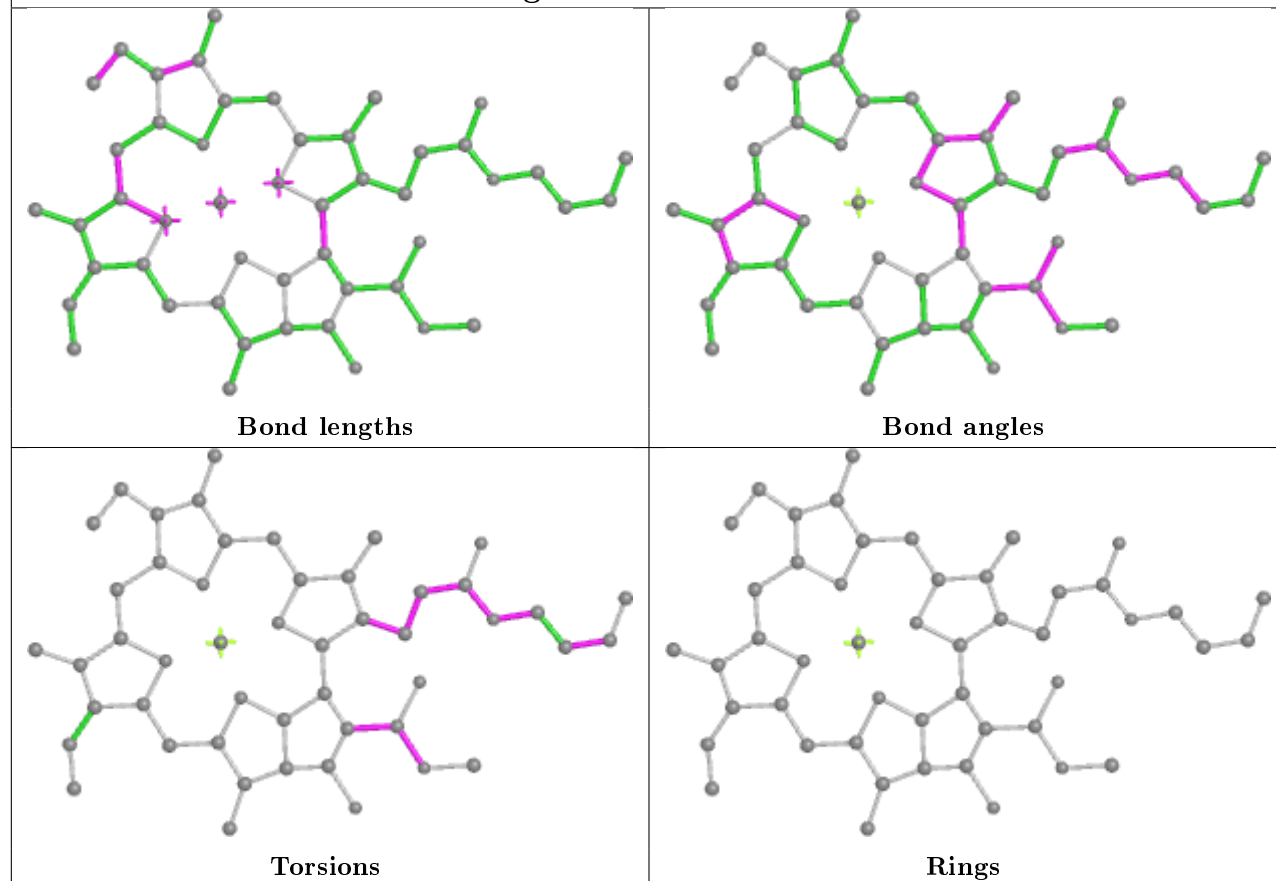
Ligand CLA B 1226



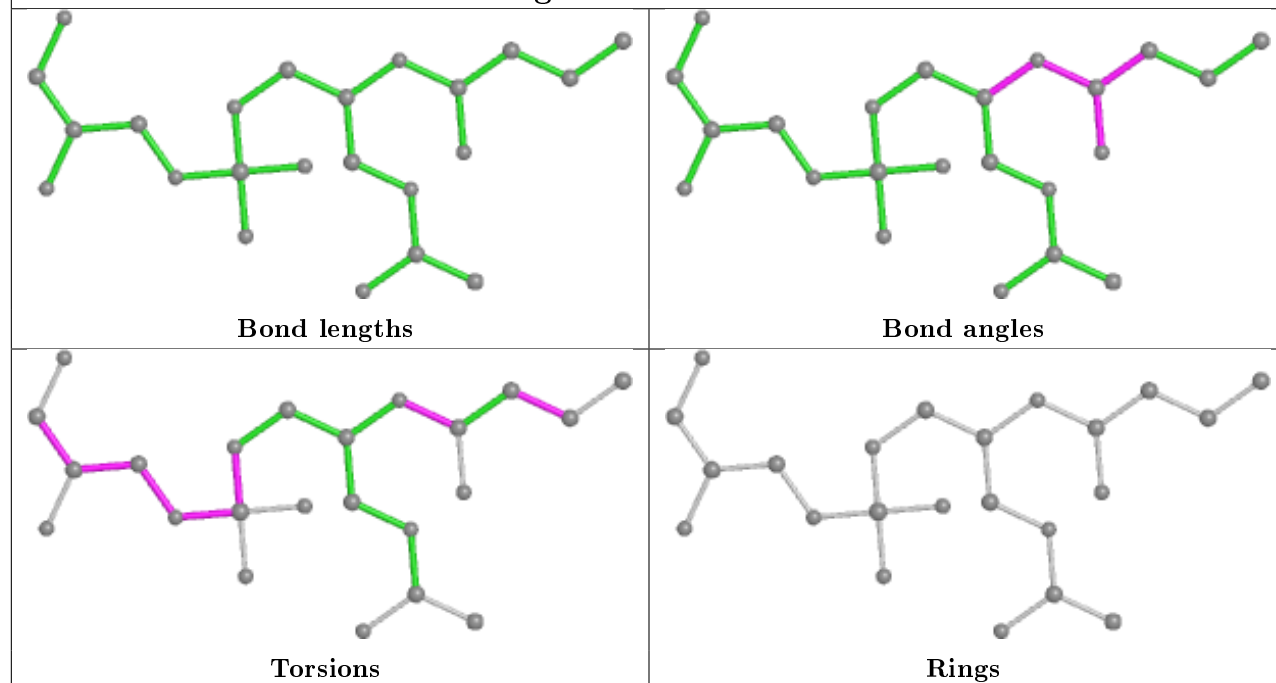
Ligand CLA B 1239



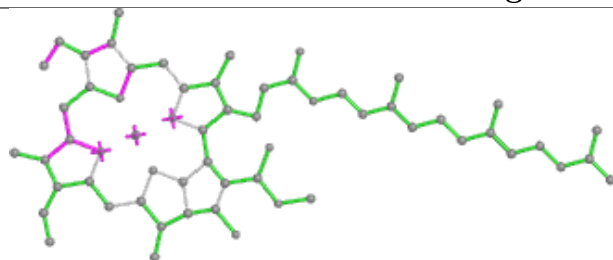
Ligand CLA B 1216



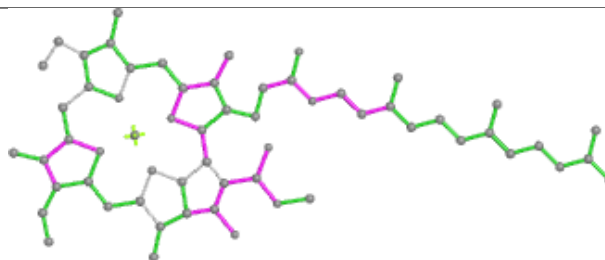
Ligand LHG 1 801



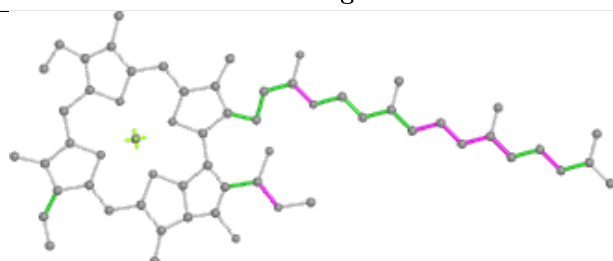
Ligand CLA A 1012



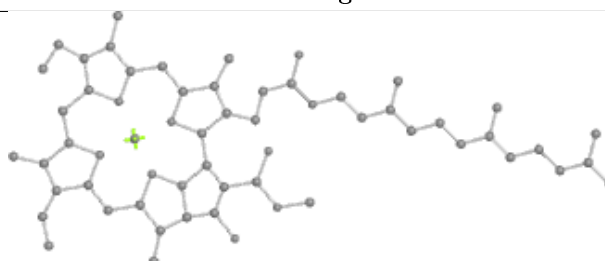
Bond lengths



Bond angles

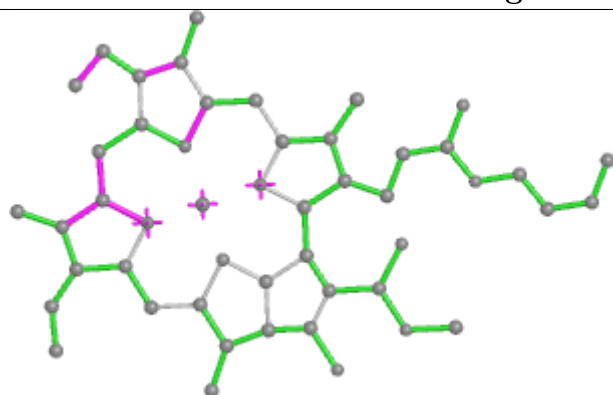


Torsions

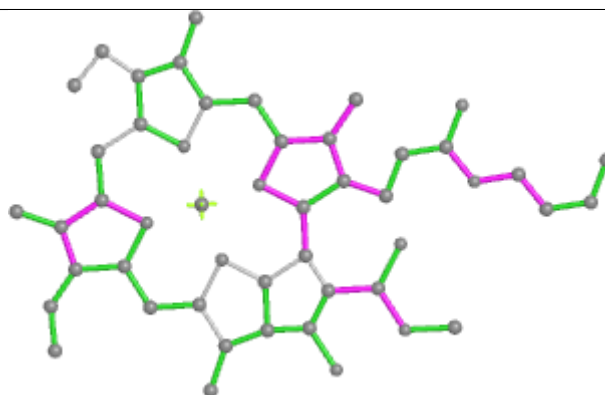


Rings

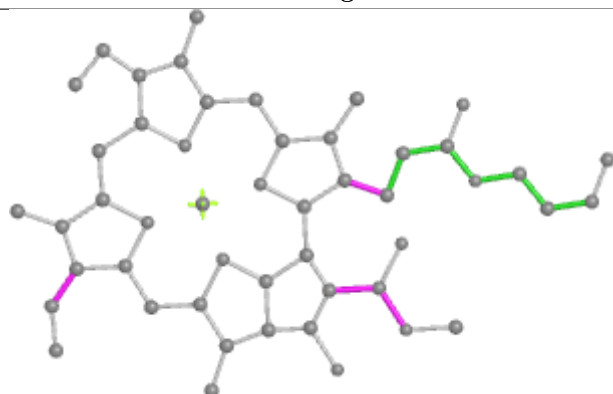
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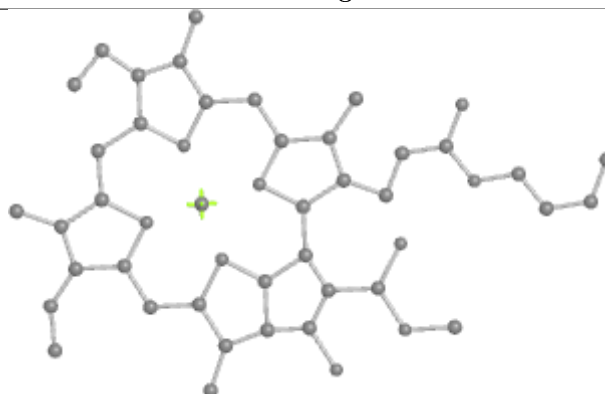
Bond lengths



Bond angles

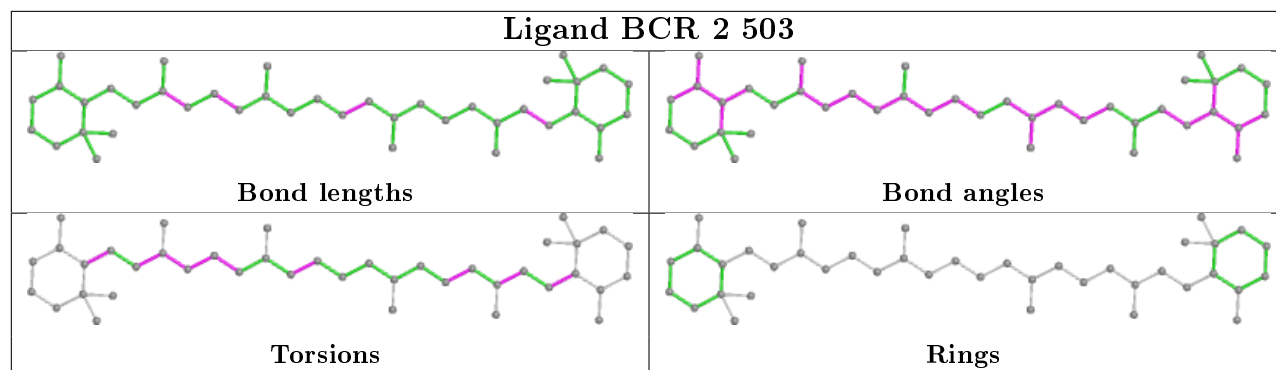


Torsions

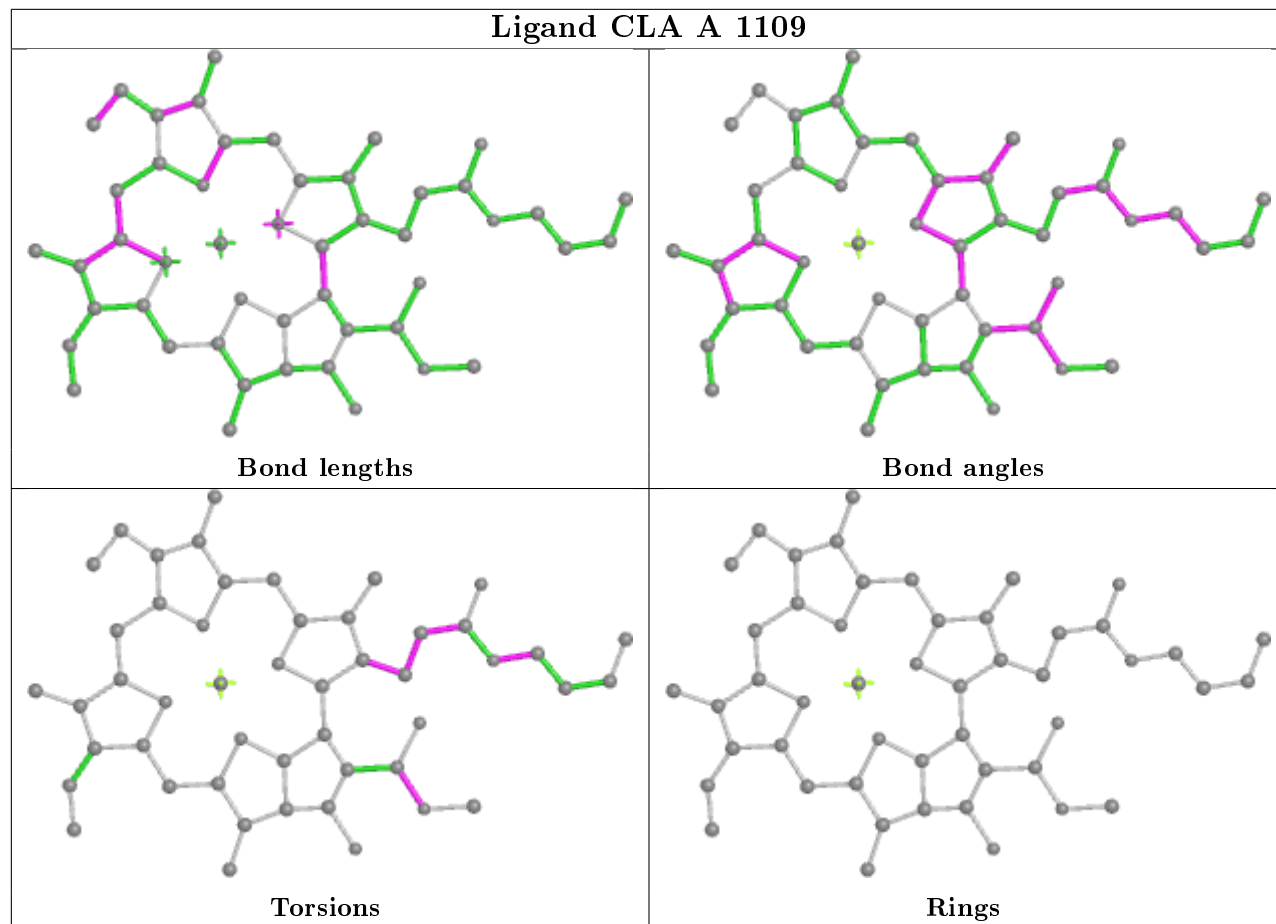


Rings

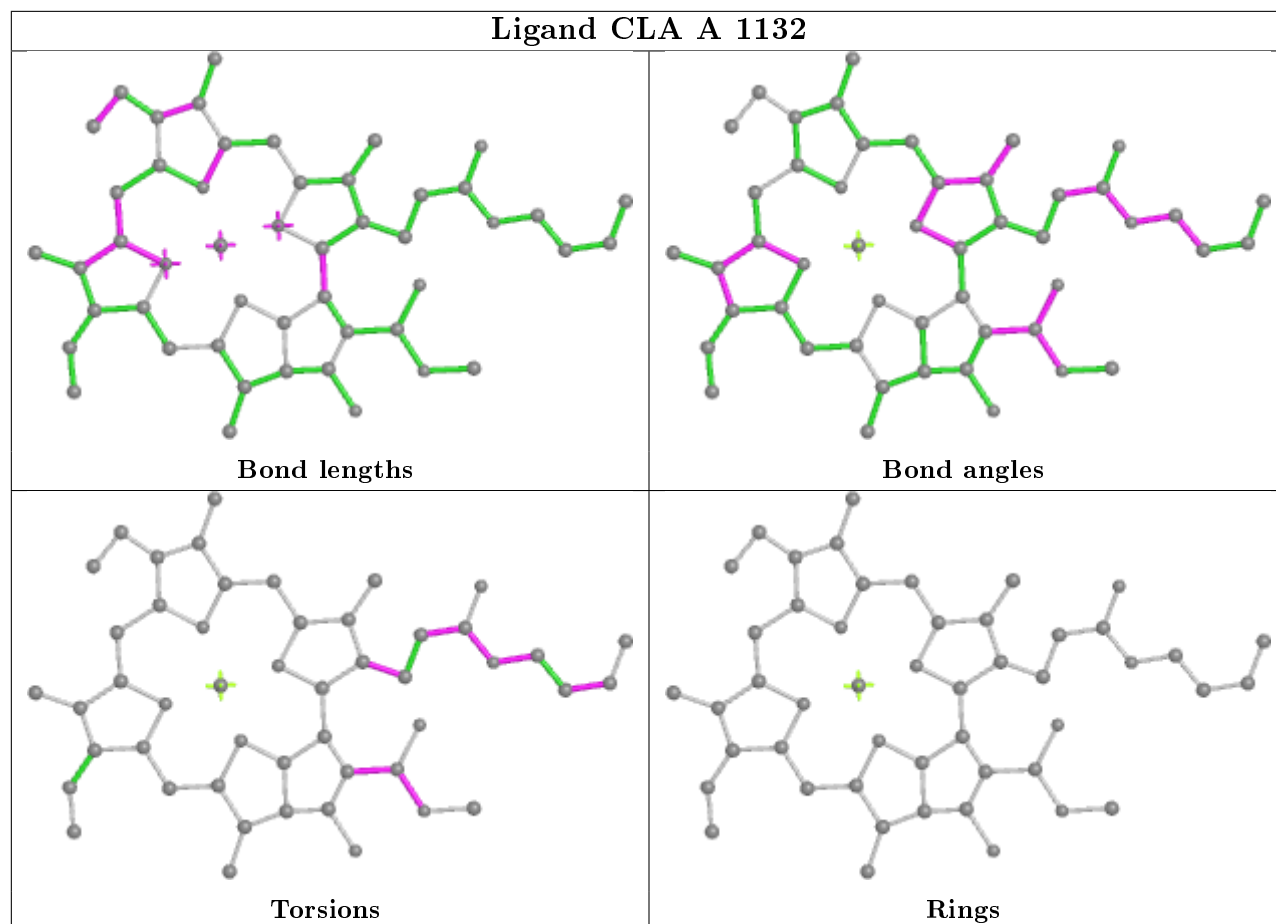
Ligand BCR 2 503



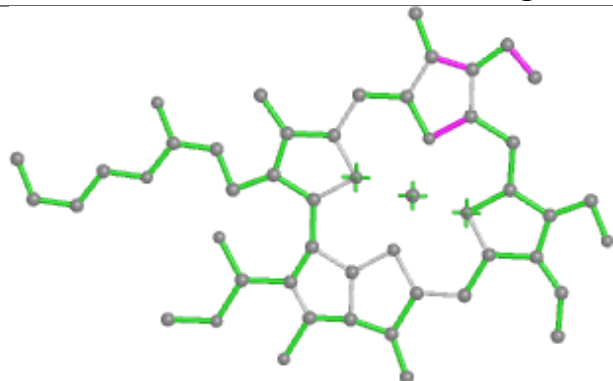
Ligand CLA A 1109



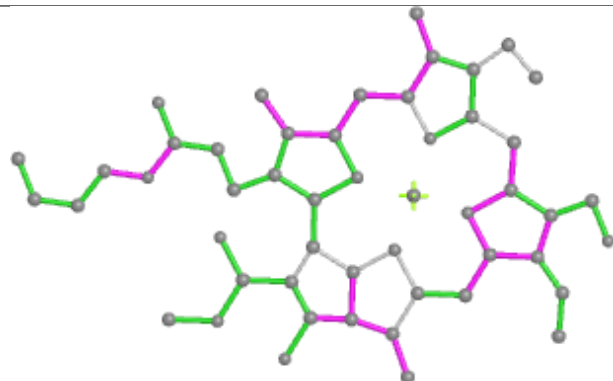
Ligand CLA A 1132



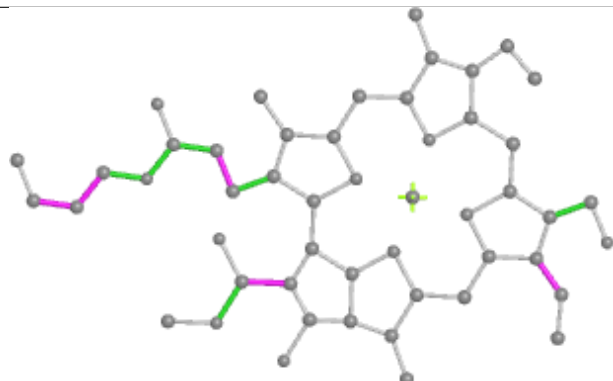
Ligand CHL 2 609



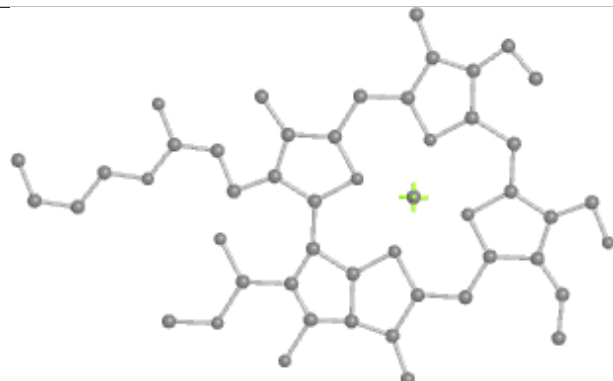
Bond lengths



Bond angles

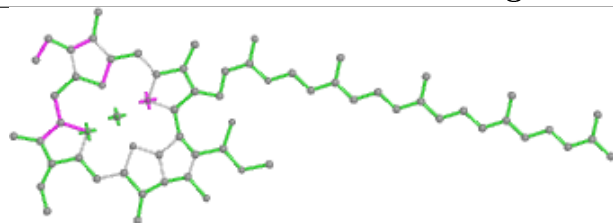


Torsions

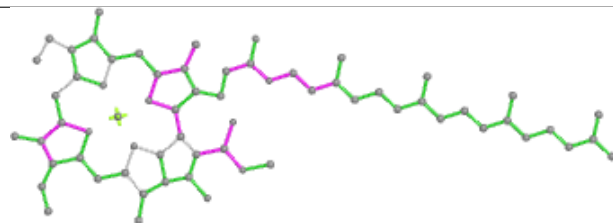


Rings

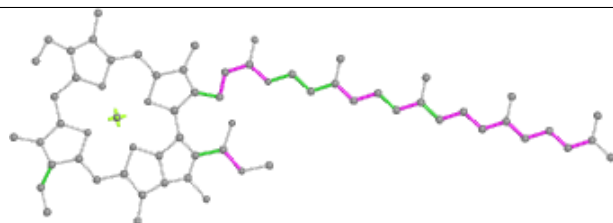
Ligand CLA B 1240



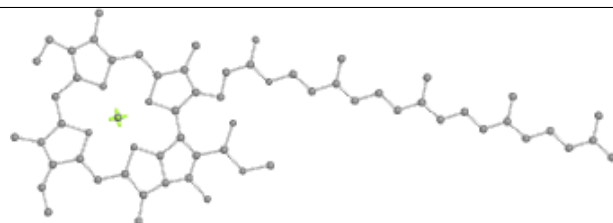
Bond lengths



Bond angles

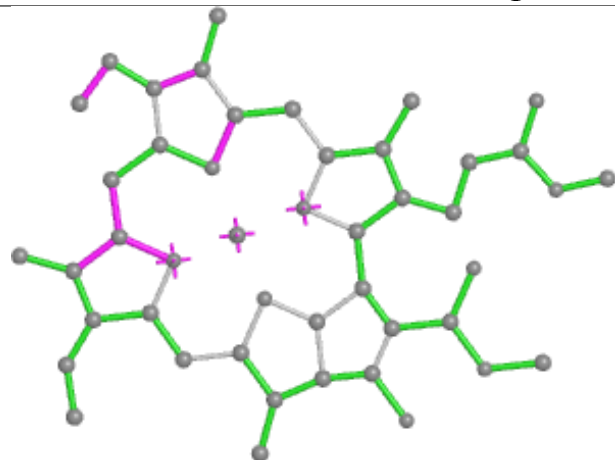


Torsions

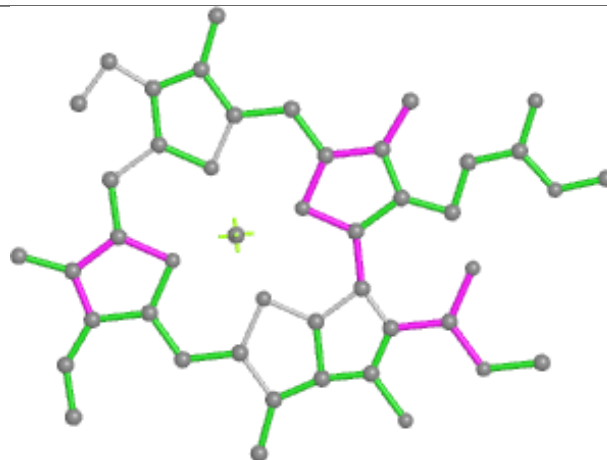


Rings

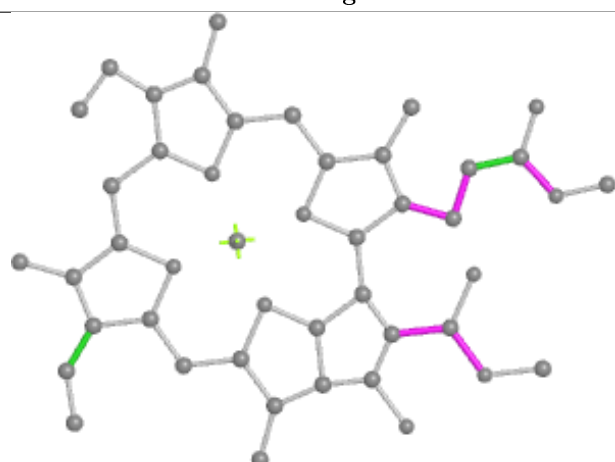
Ligand CLA B 1217



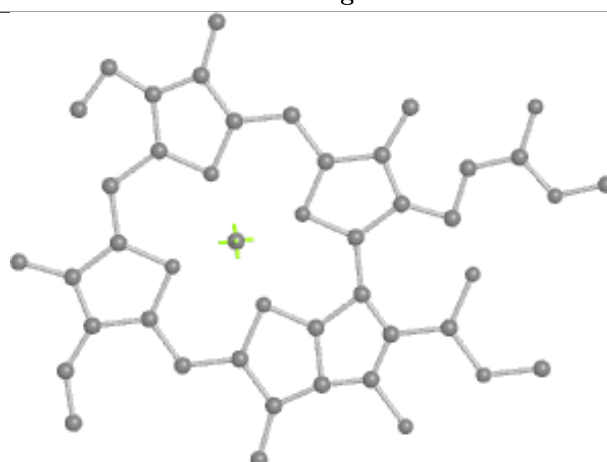
Bond lengths



Bond angles

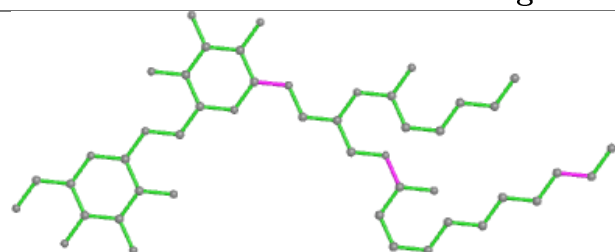


Torsions

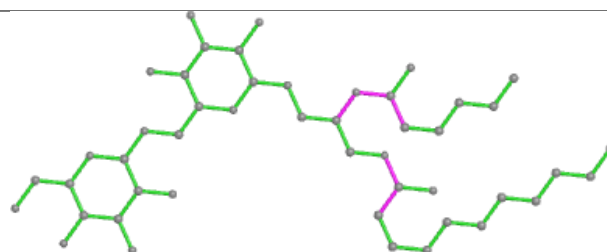


Rings

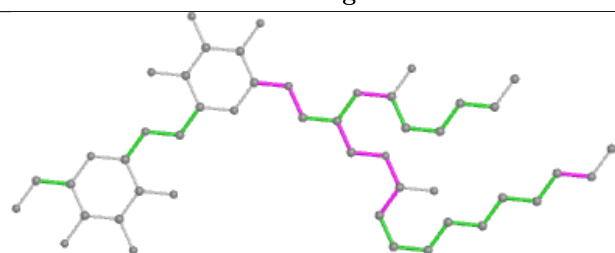
Ligand DGD 2 811



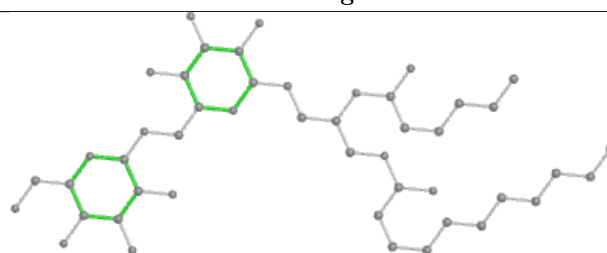
Bond lengths



Bond angles

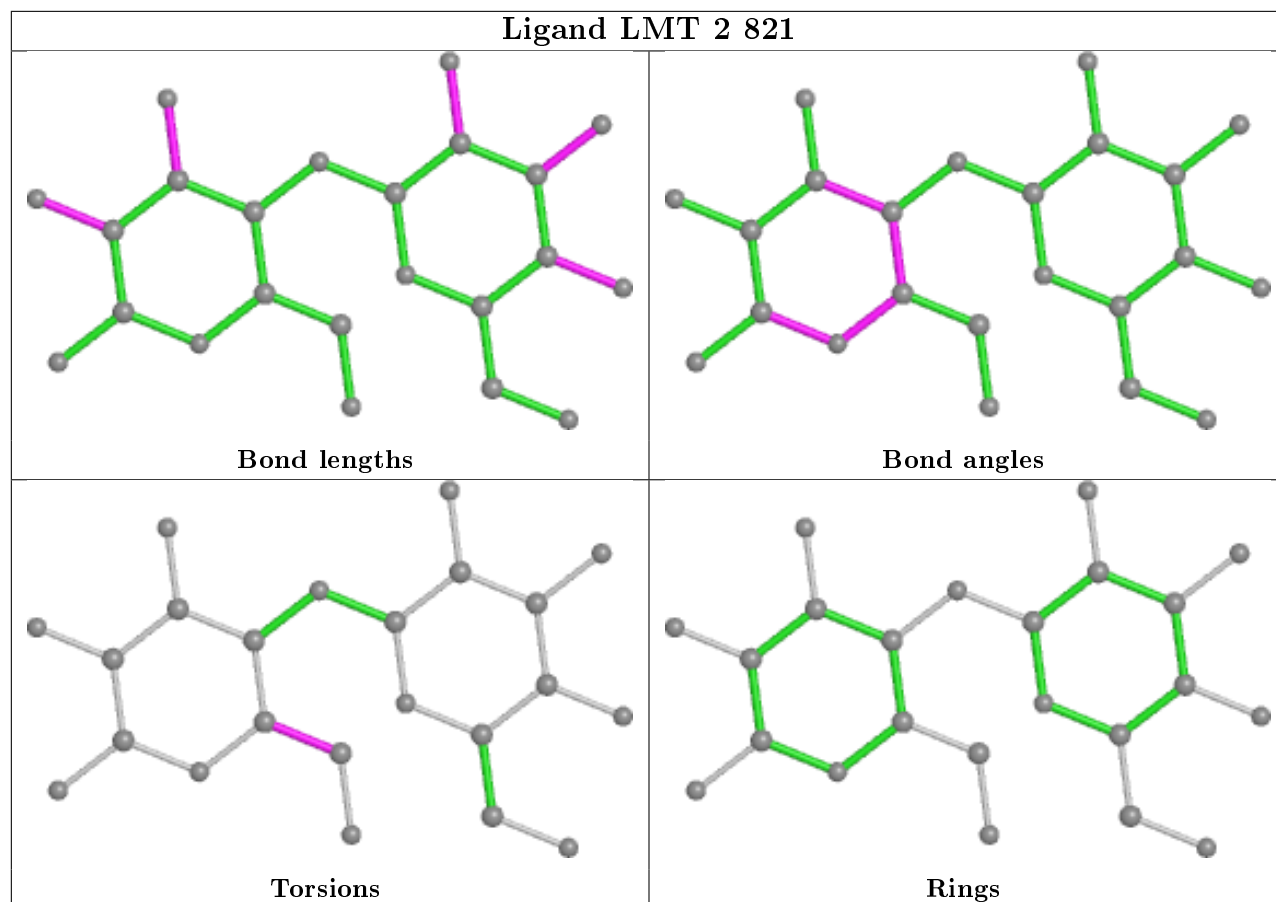


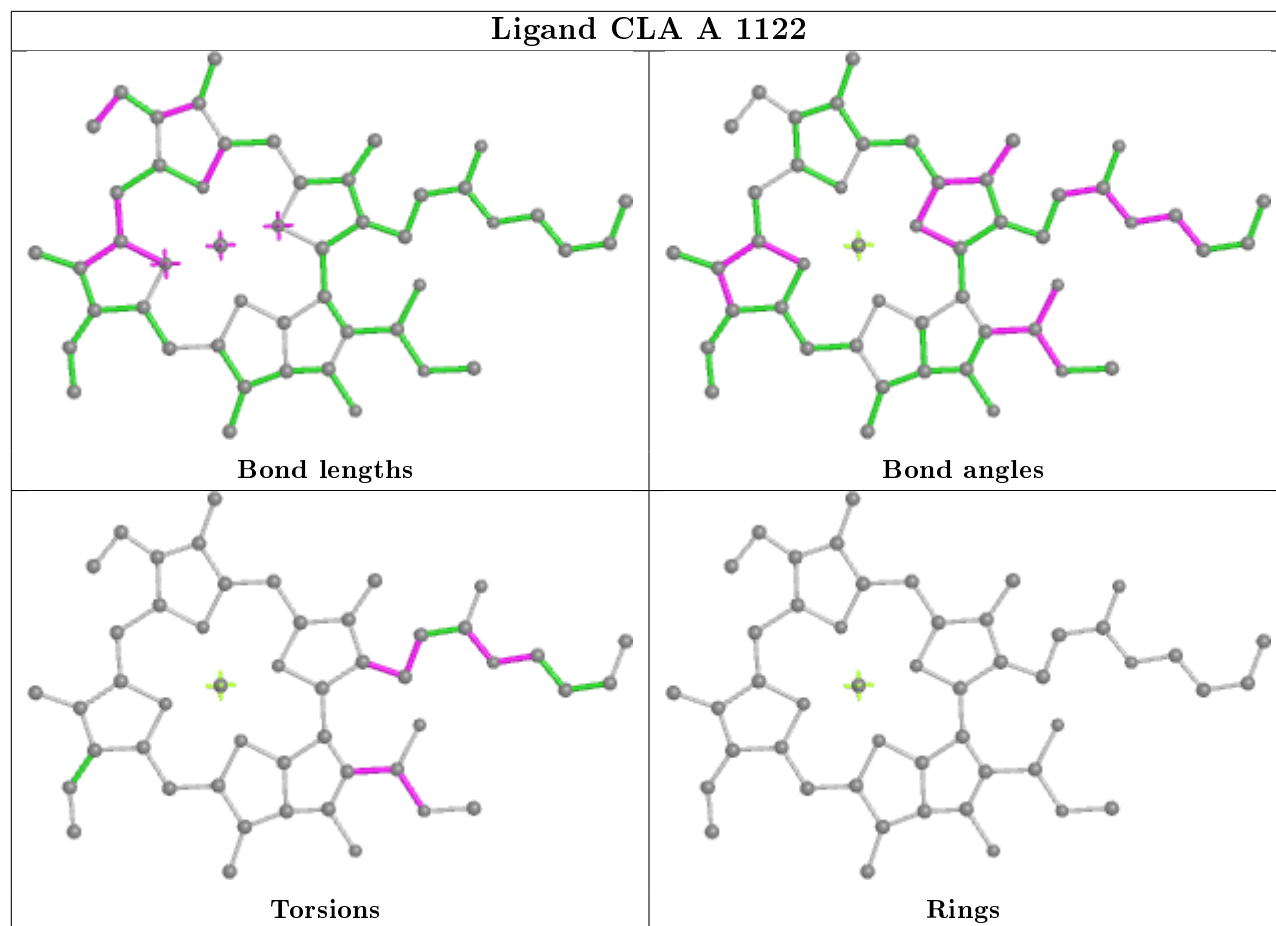
Torsions

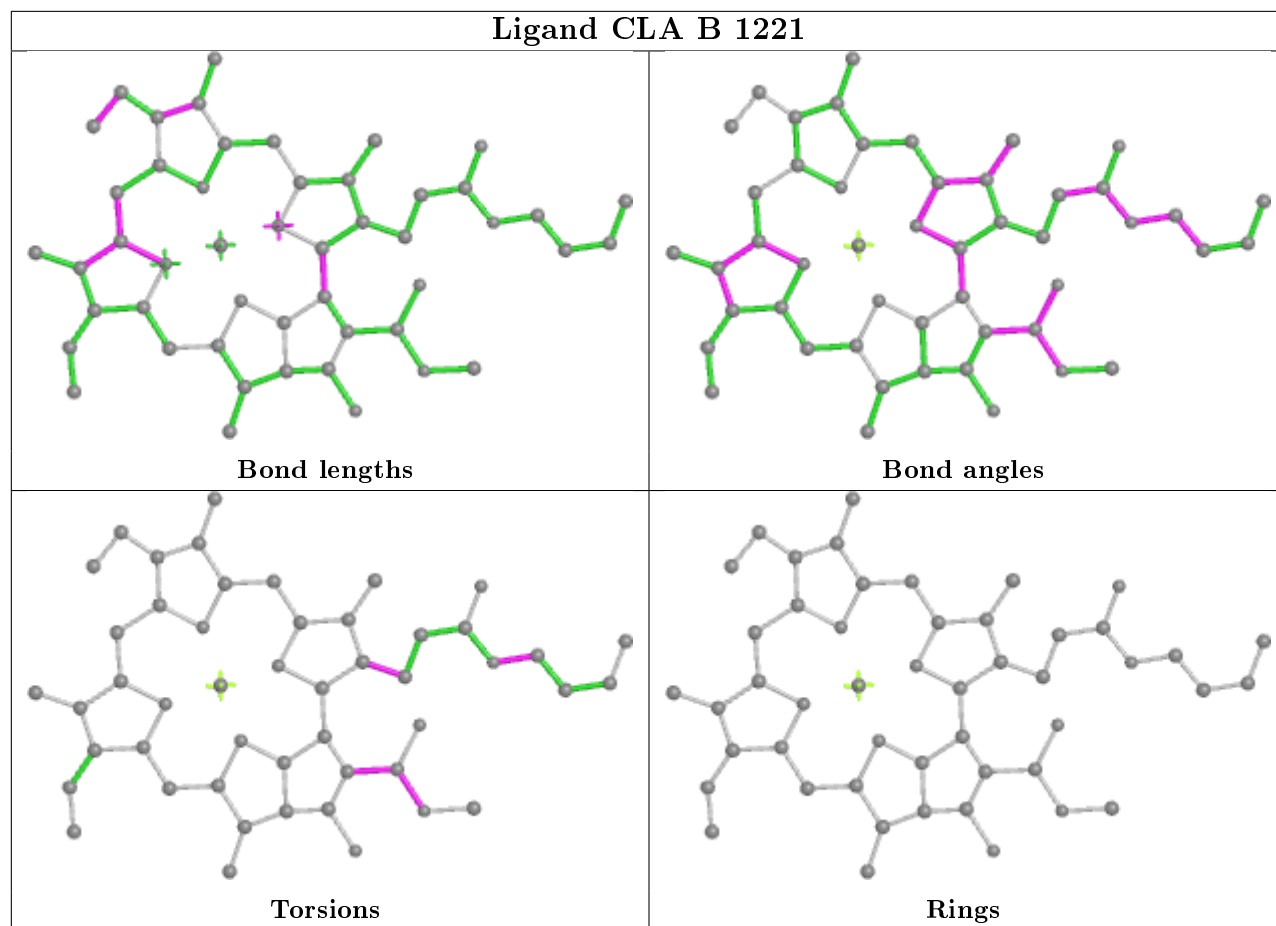


Rings

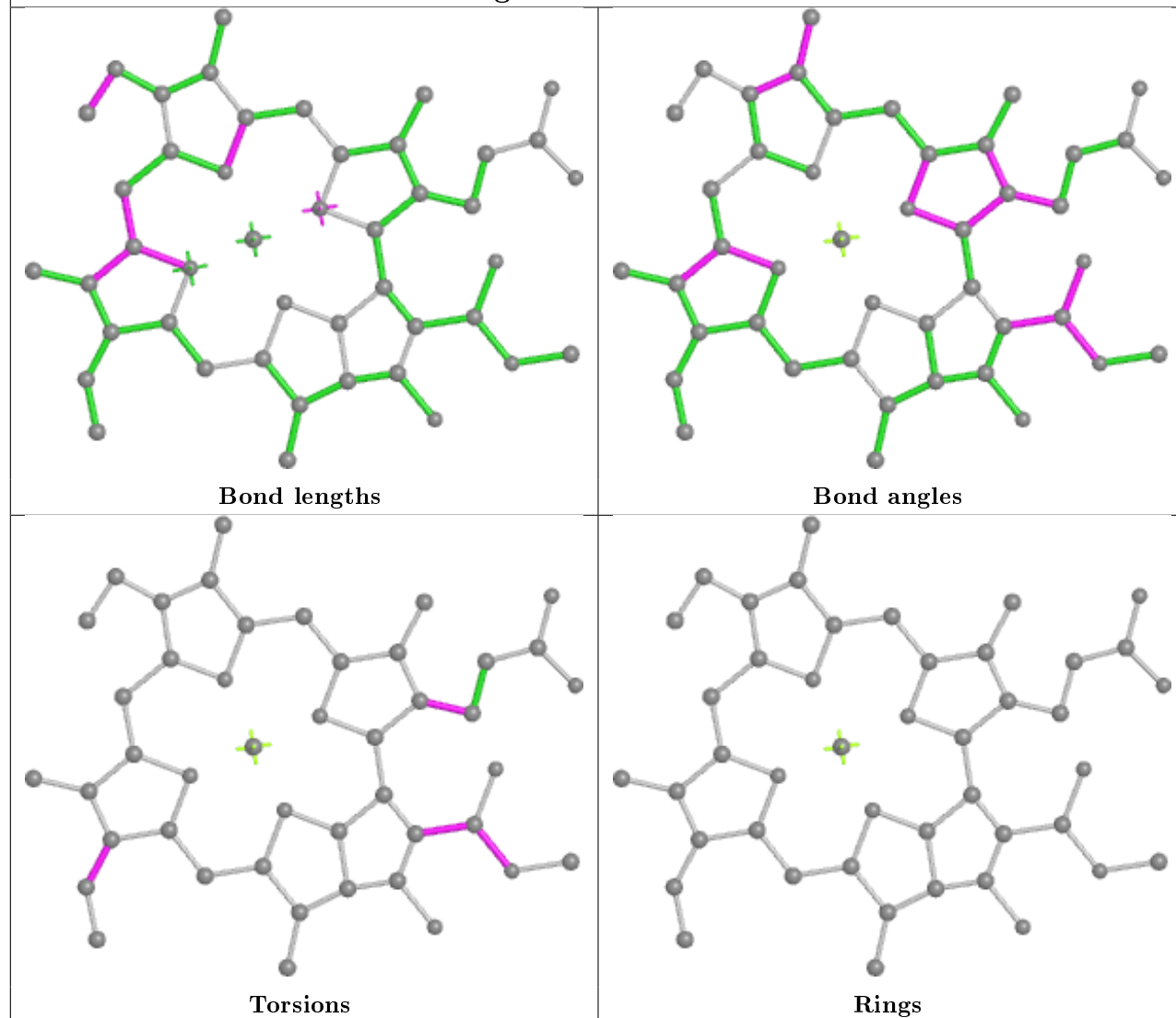
Ligand LMT 2 821



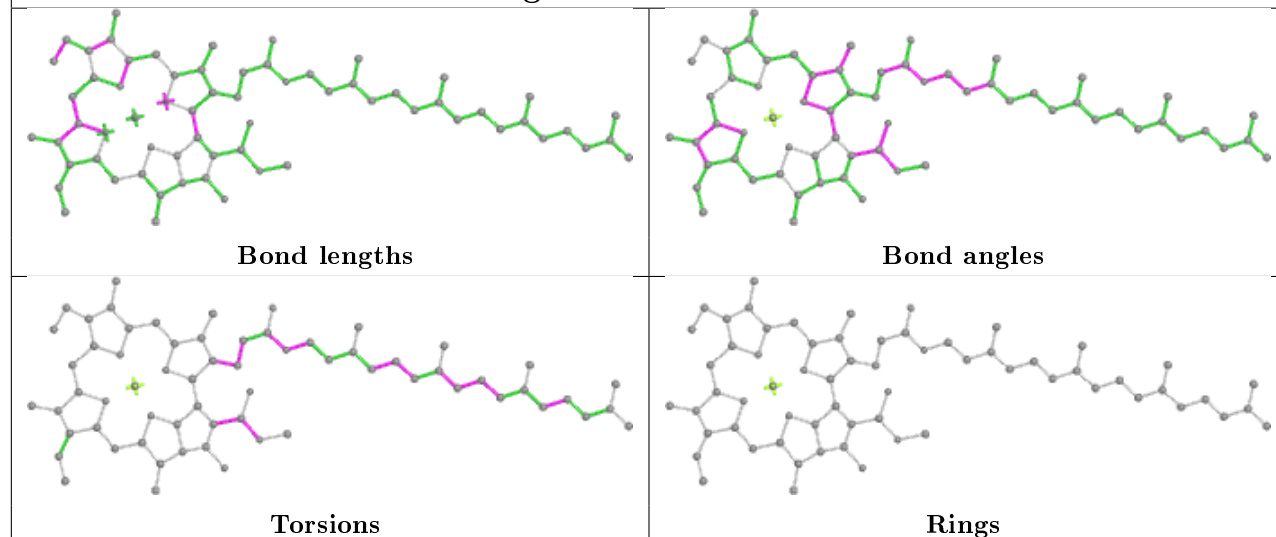


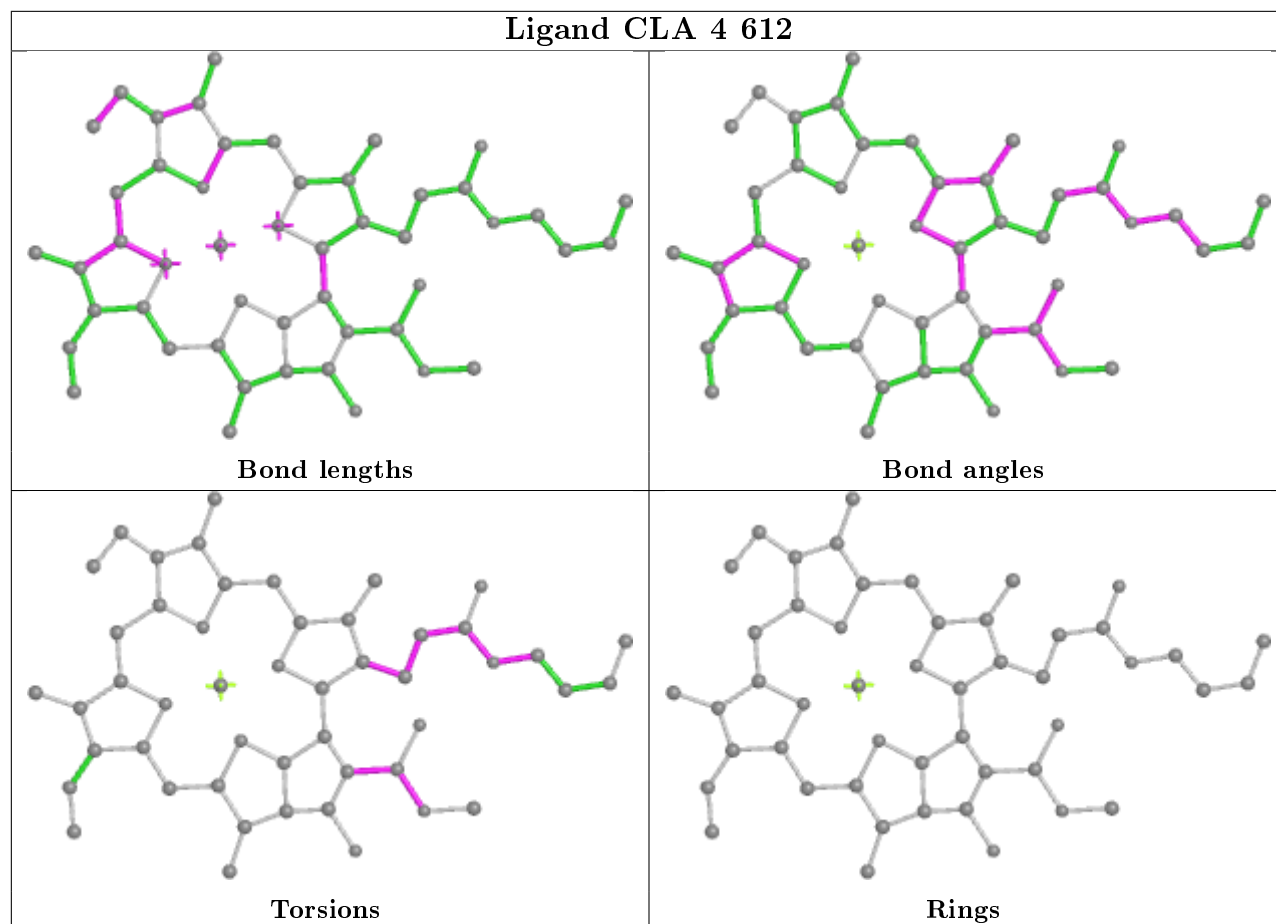
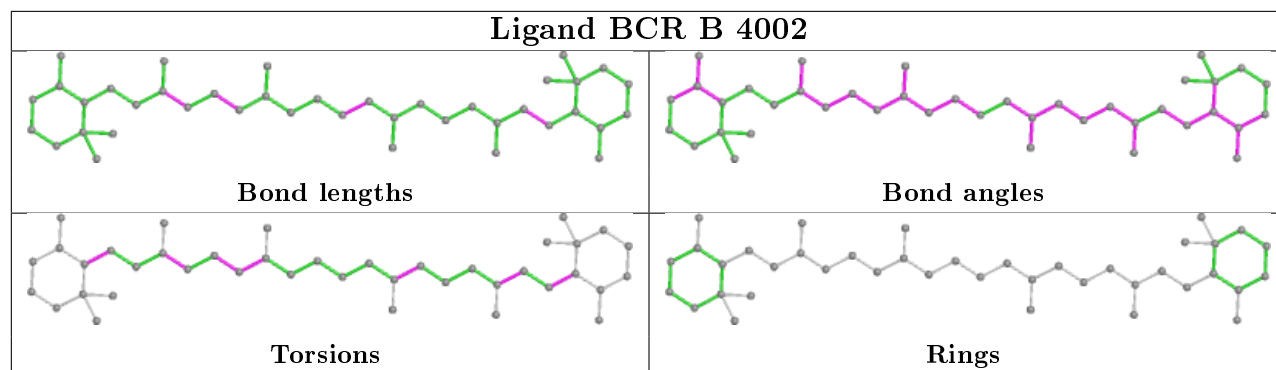


Ligand CLA 1 606

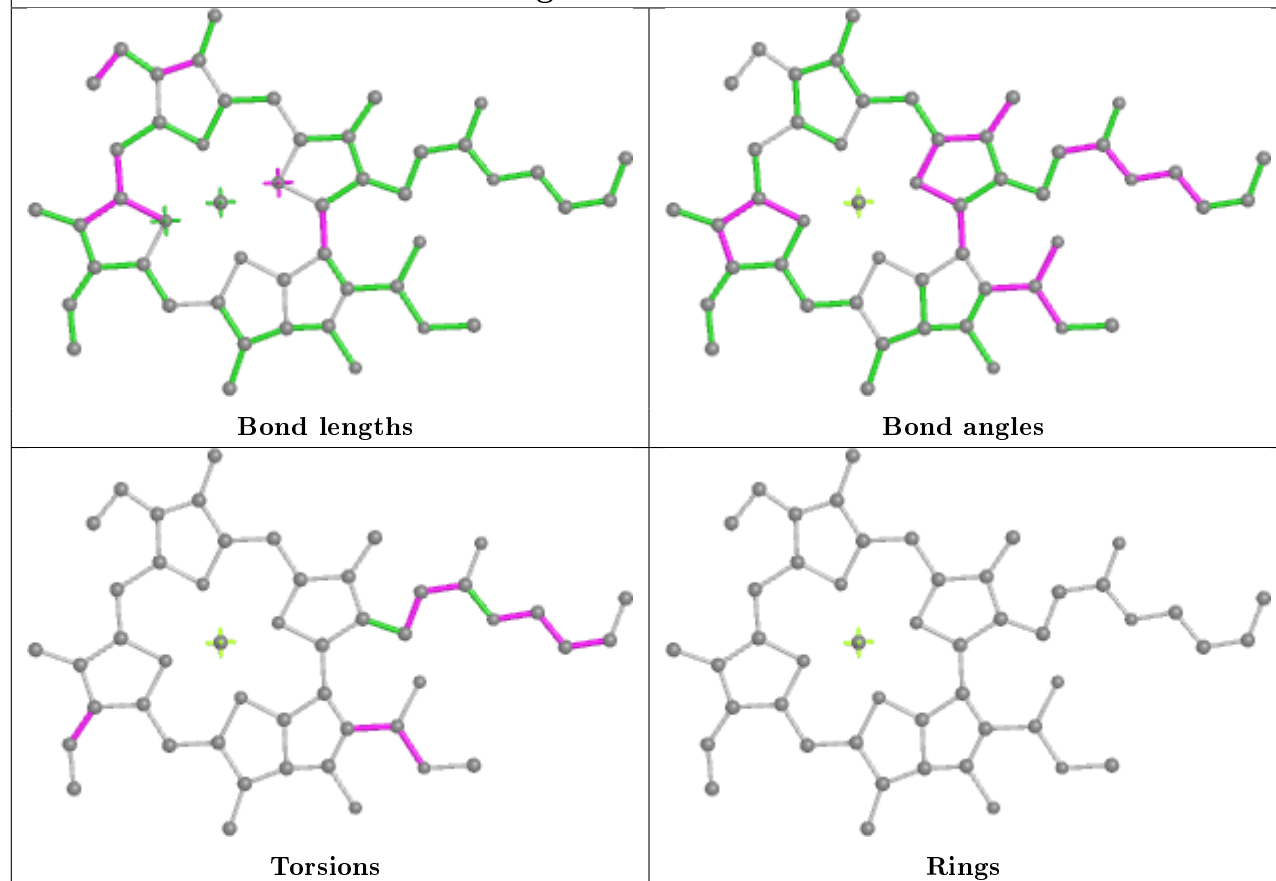


Ligand CLA B 1021

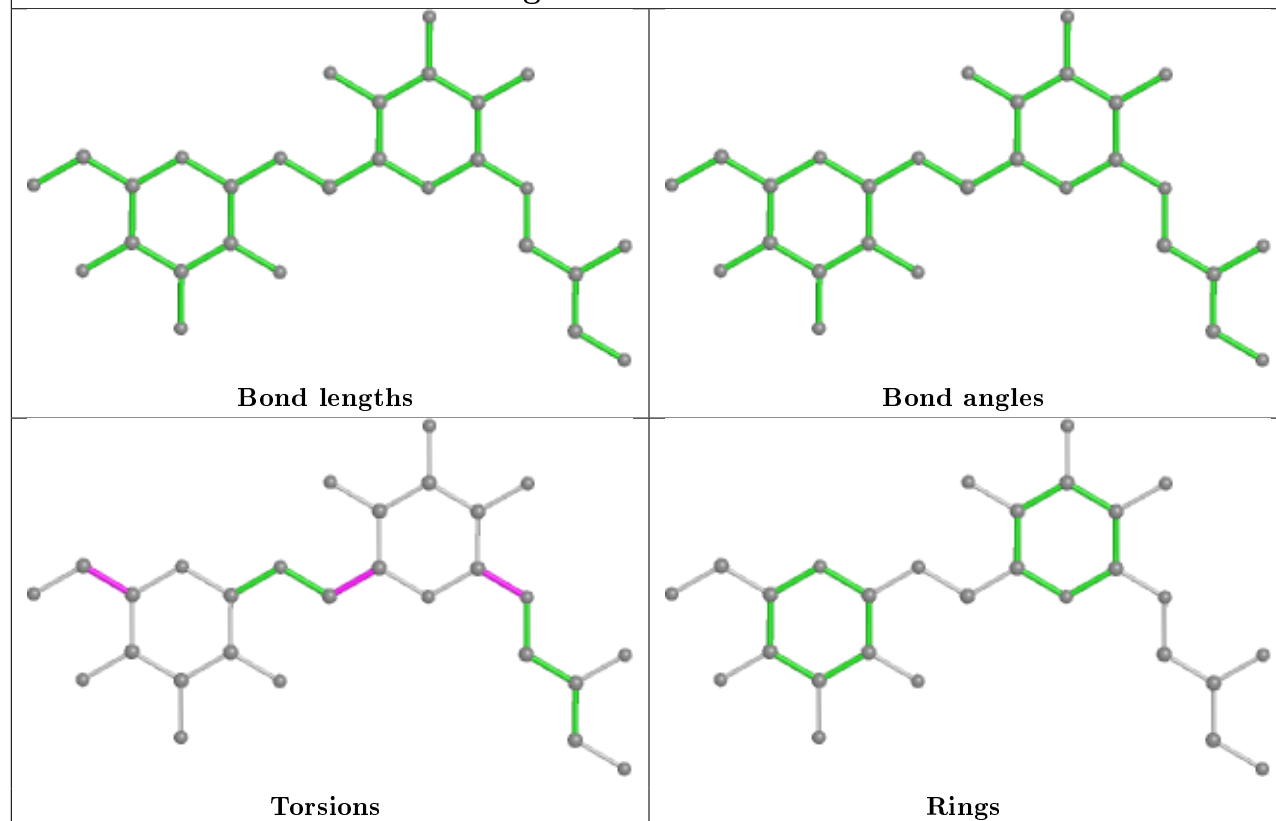




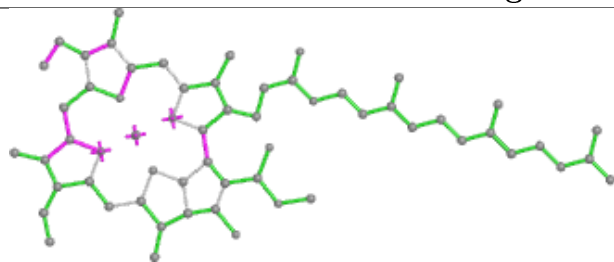
Ligand CLA 1 611



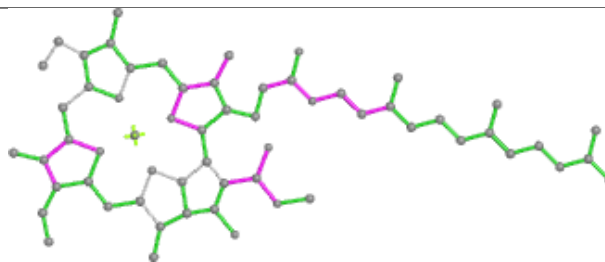
Ligand DGD J 5001



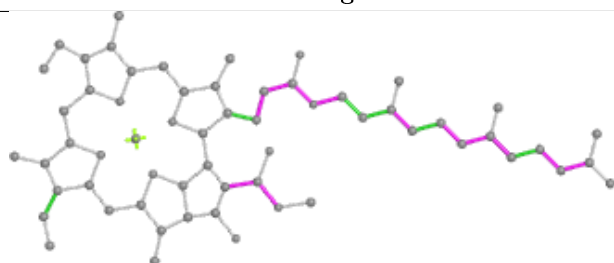
Ligand CLA B 1235



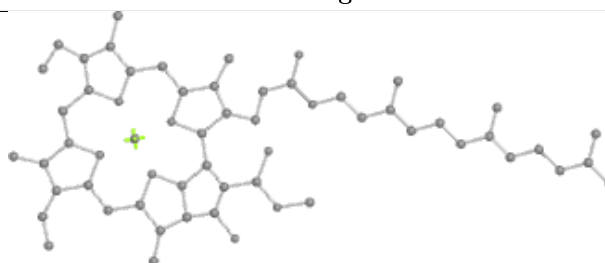
Bond lengths



Bond angles

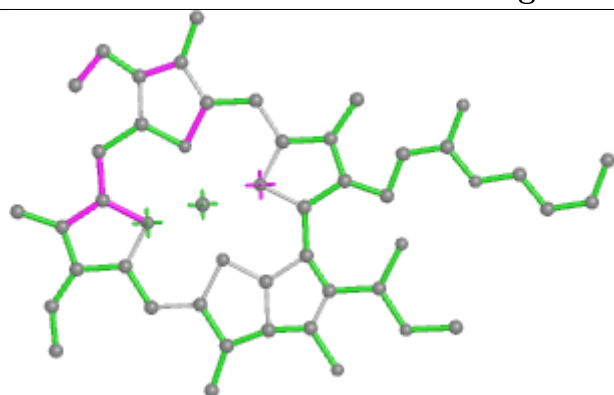


Torsions

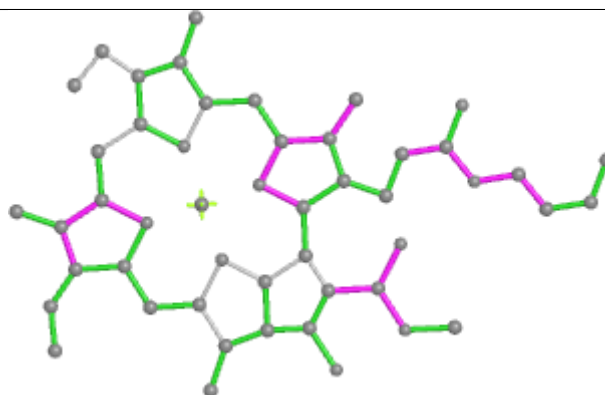


Rings

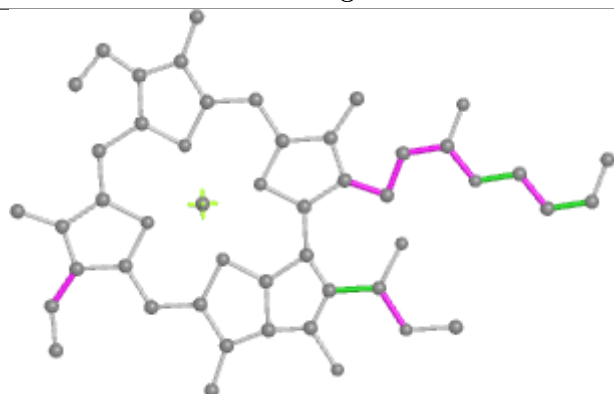
Ligand CLA 3 601



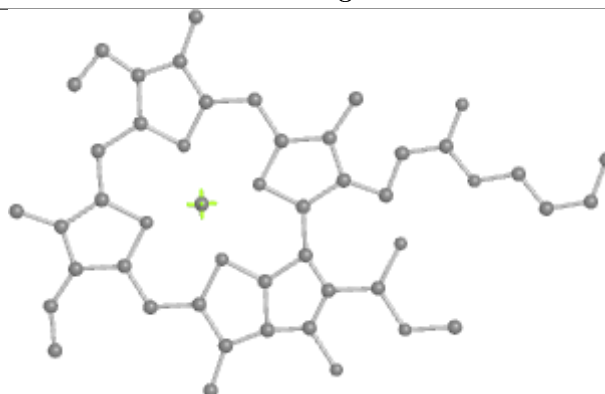
Bond lengths



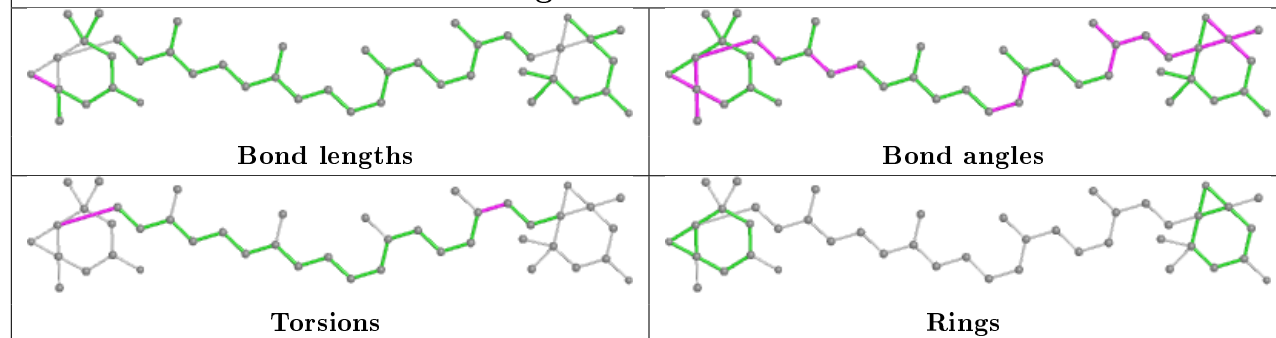
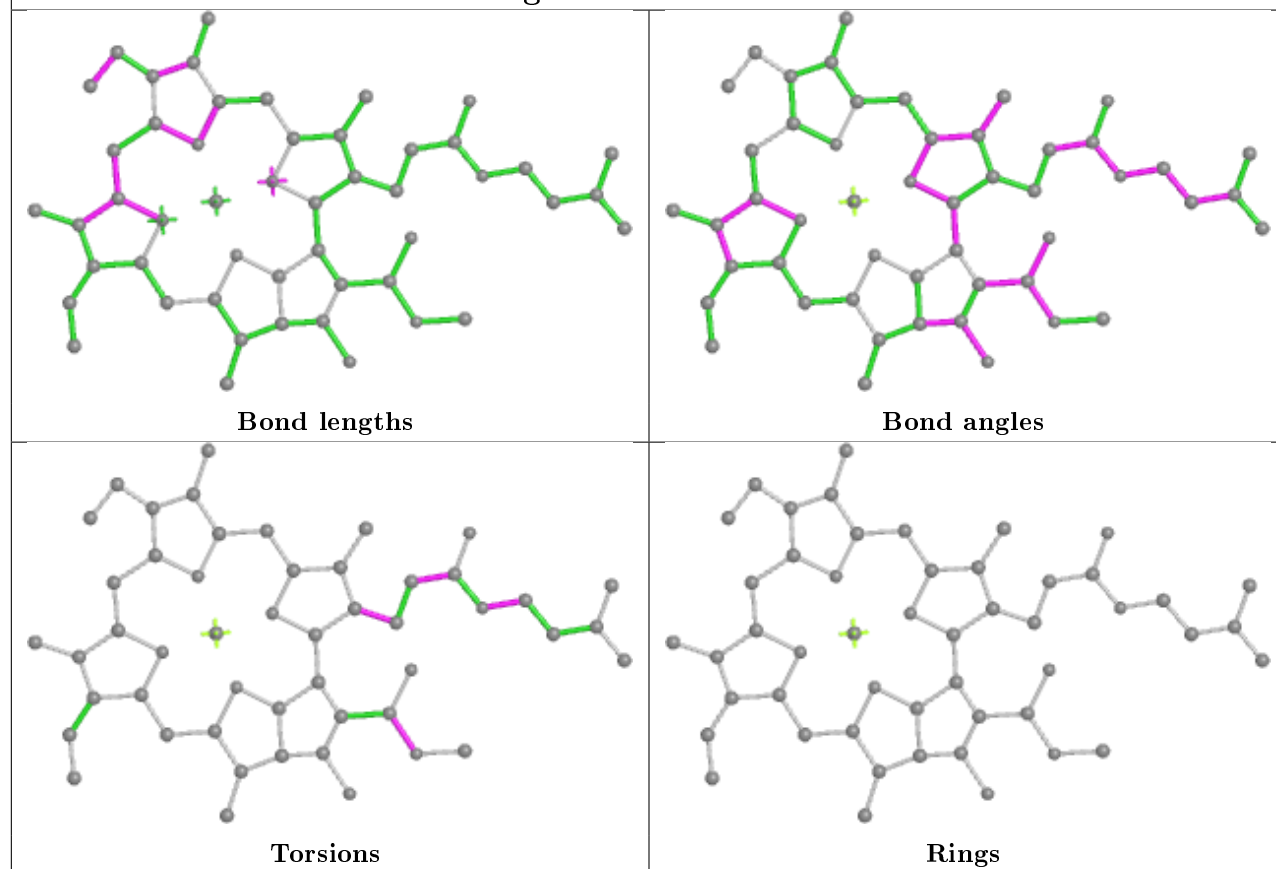
Bond angles

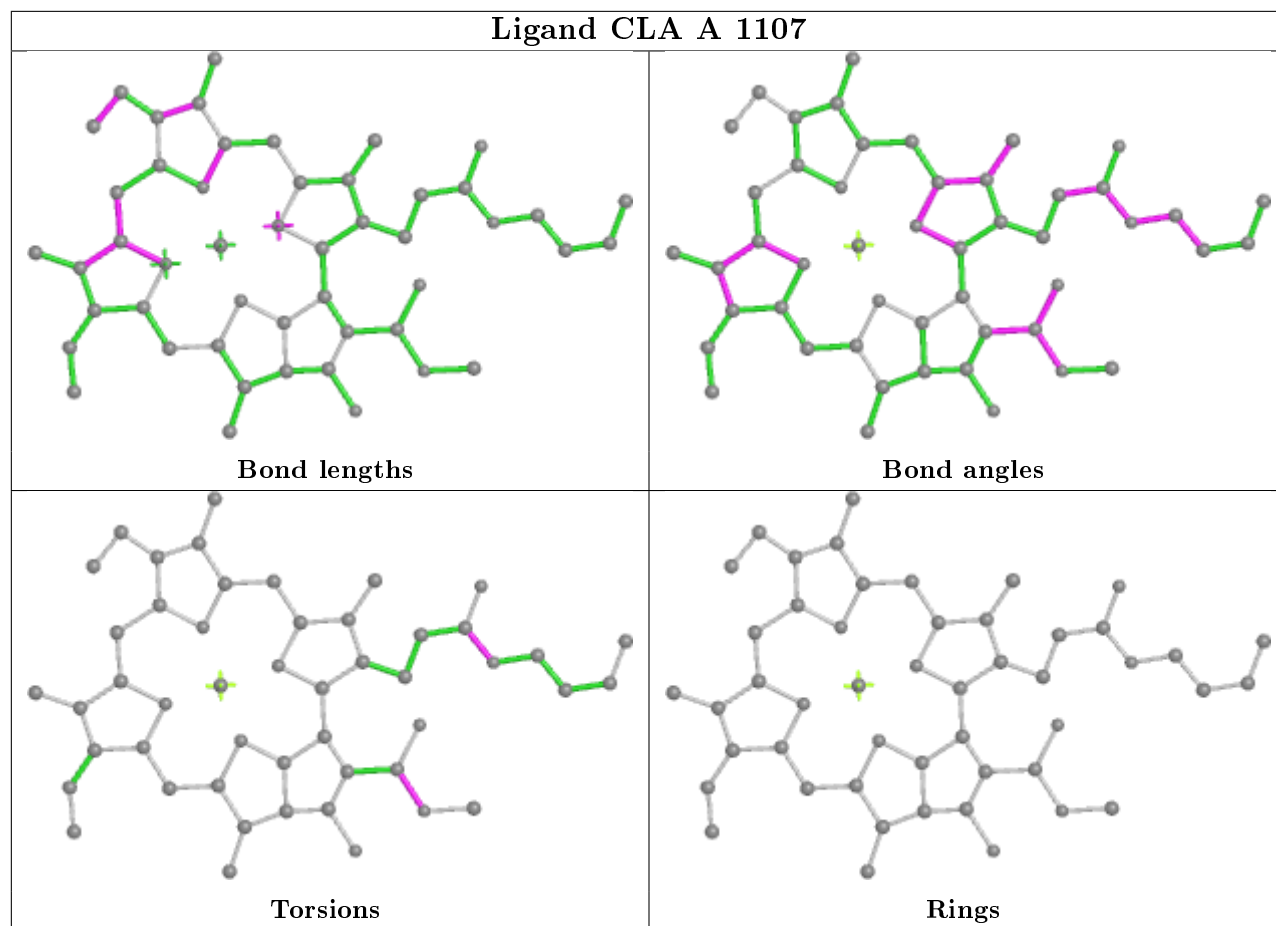


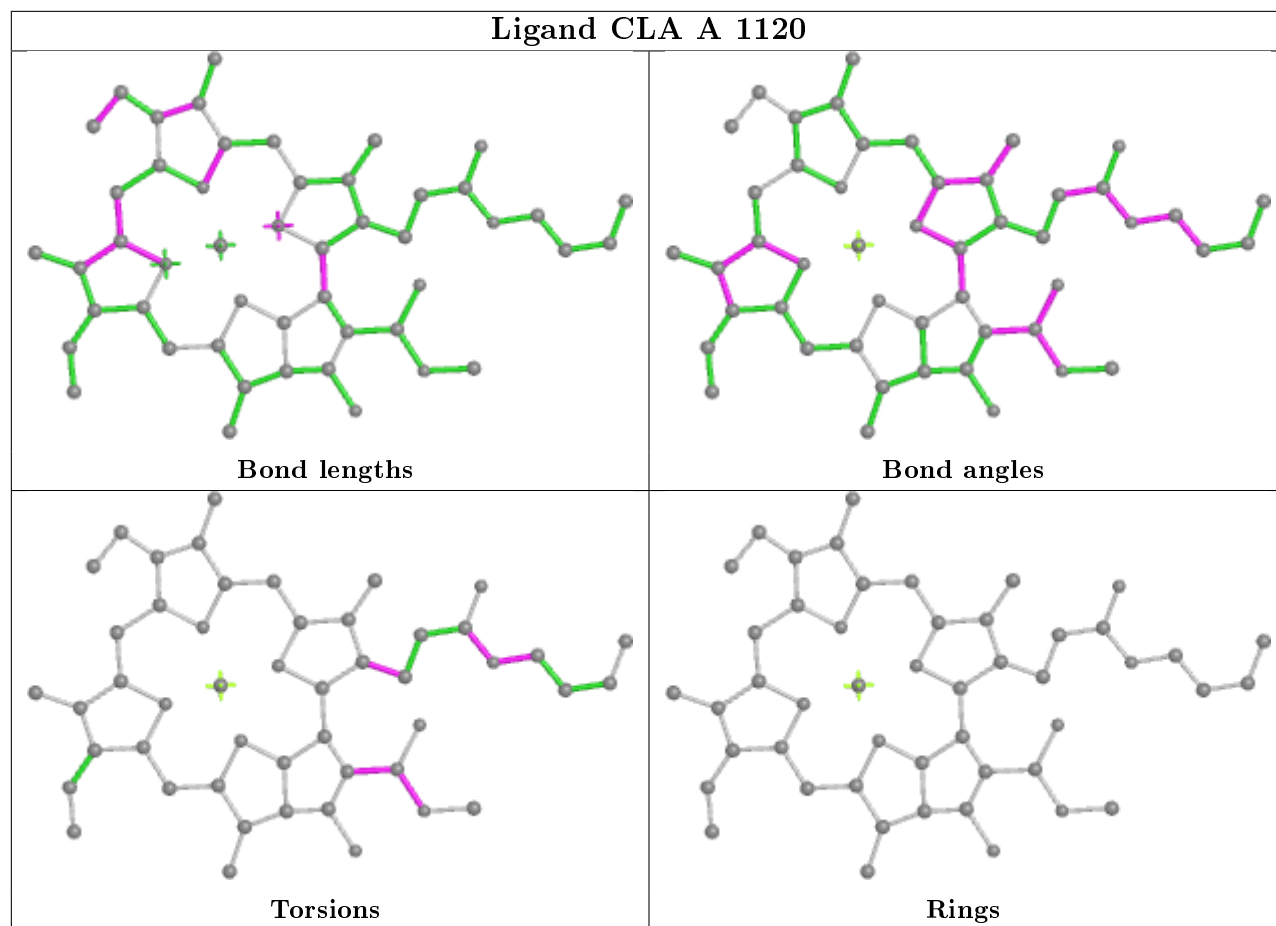
Torsions



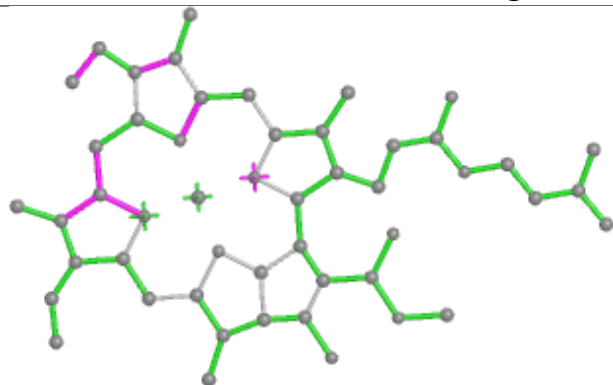
Rings

Ligand XAT 2 502**Ligand CLA B 1223**

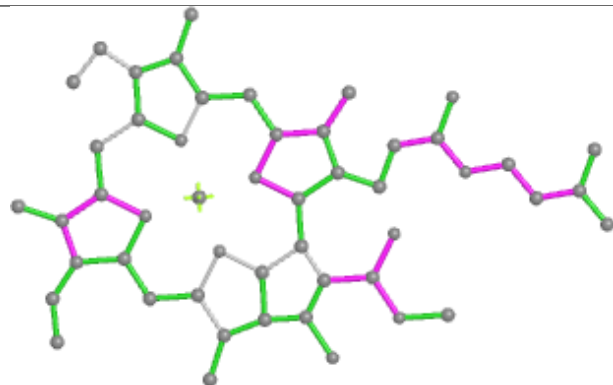




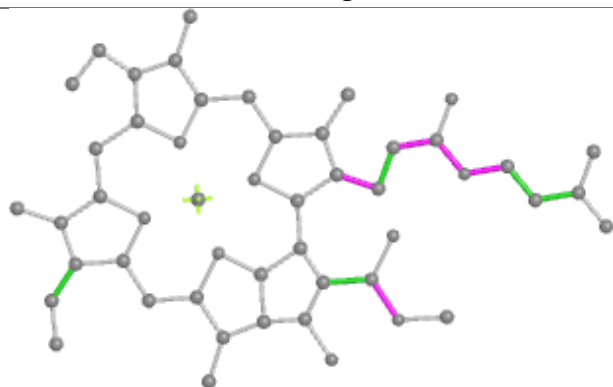
Ligand CLA A 1141



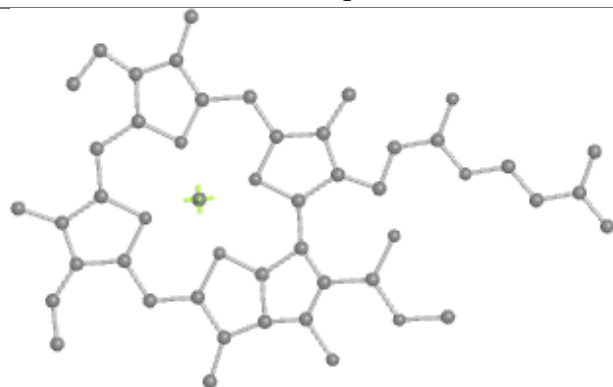
Bond lengths



Bond angles

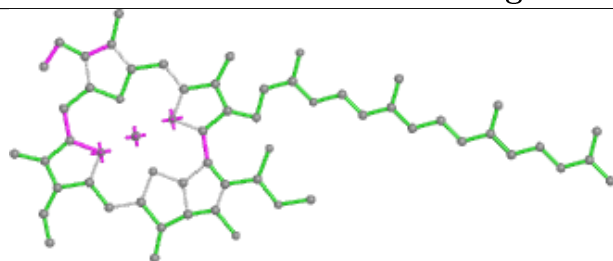


Torsions

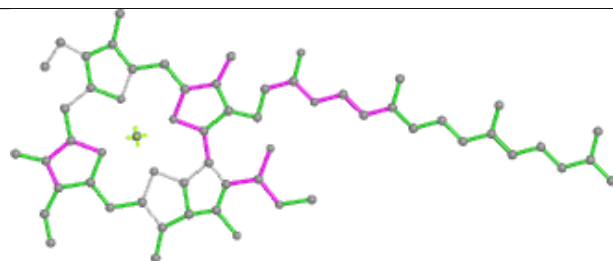


Rings

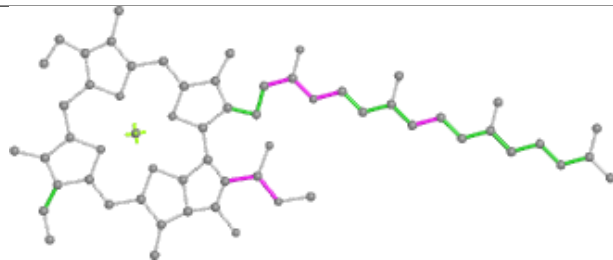
Ligand CLA B 1228



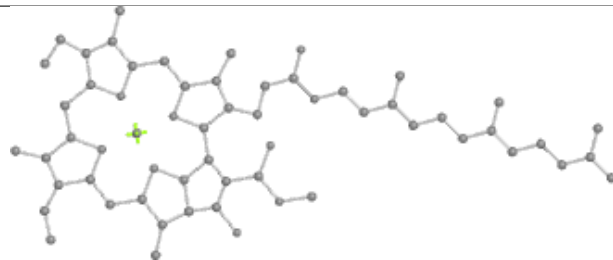
Bond lengths



Bond angles

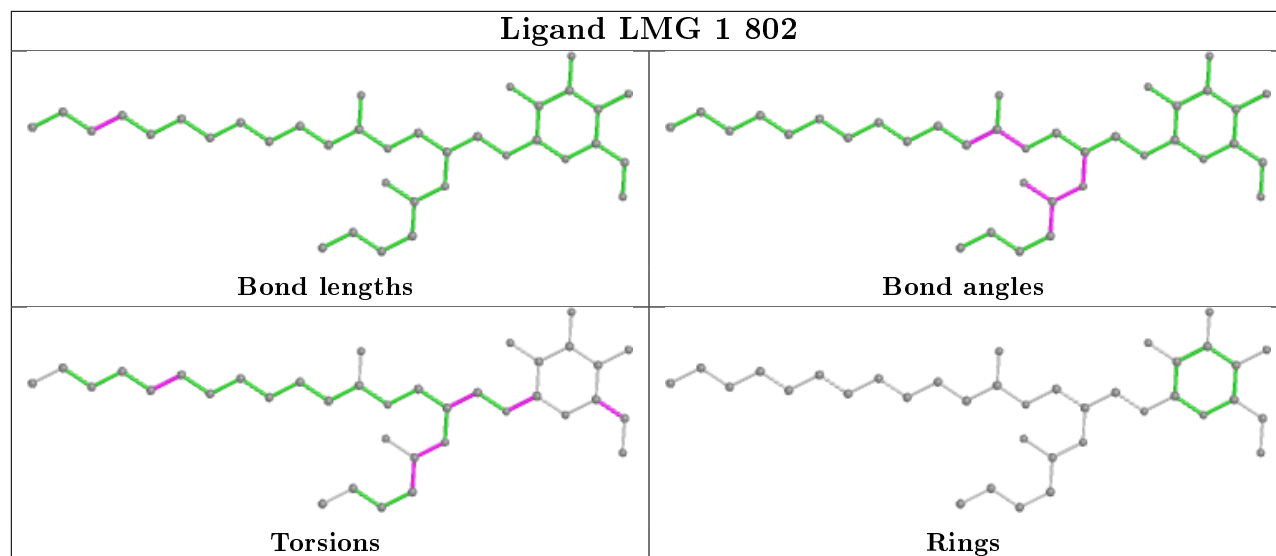


Torsions

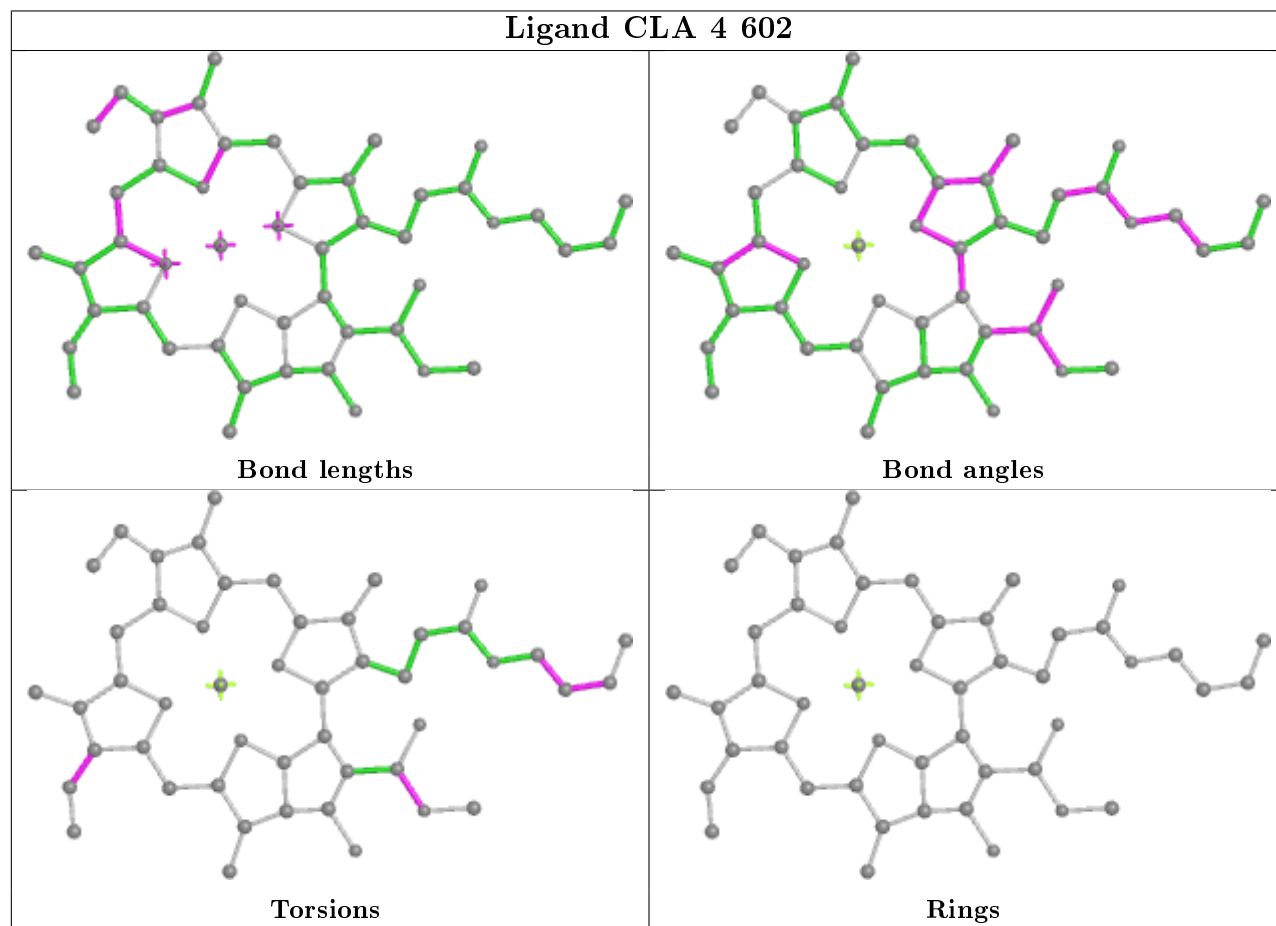


Rings

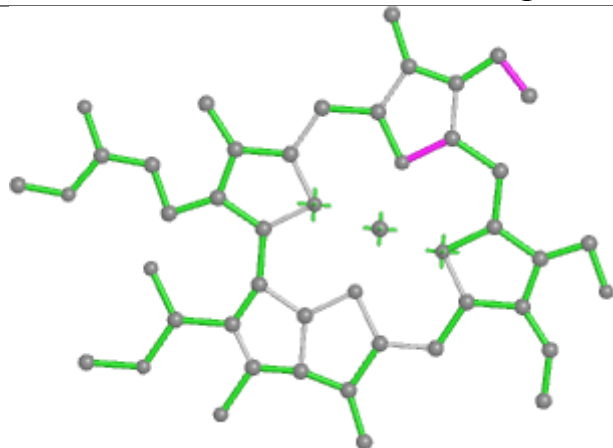
Ligand LMG 1 802



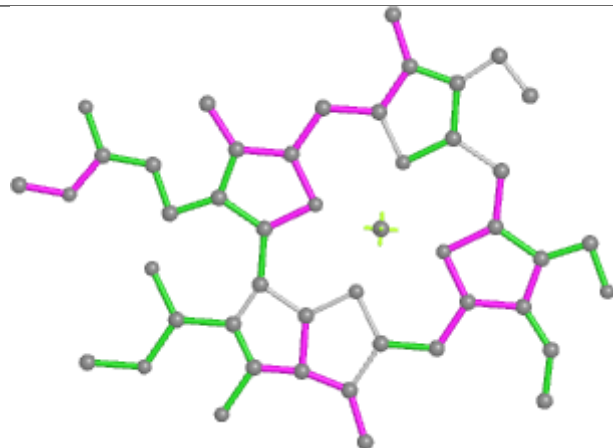
Ligand CLA 4 602



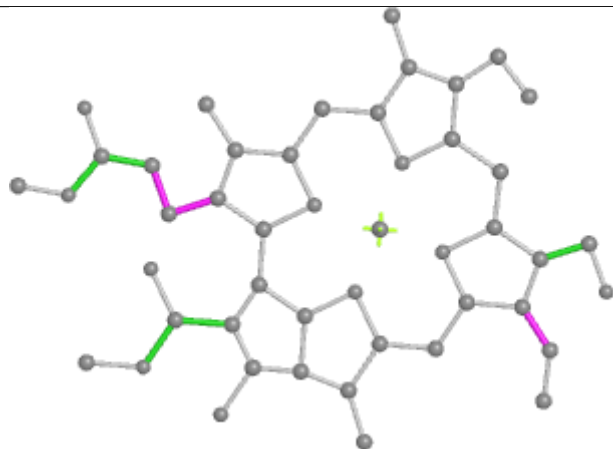
Ligand CHL 1 610



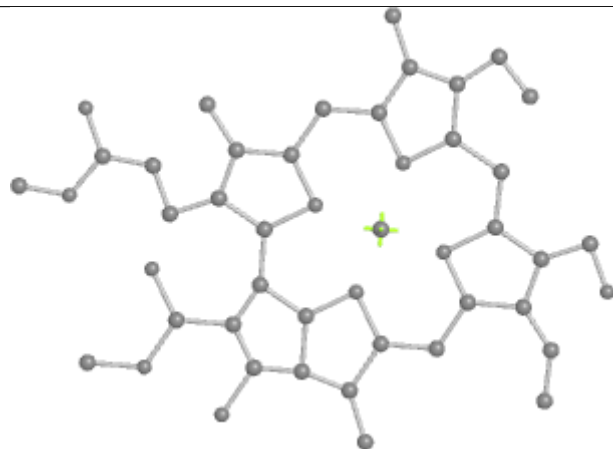
Bond lengths



Bond angles

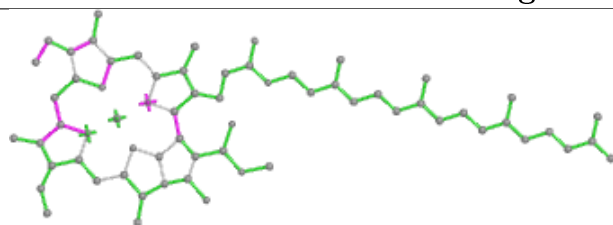


Torsions

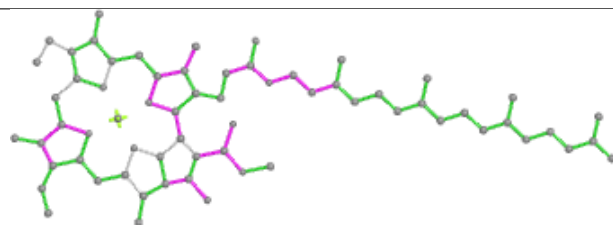


Rings

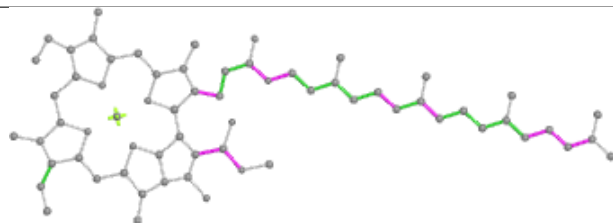
Ligand CLA 2 605



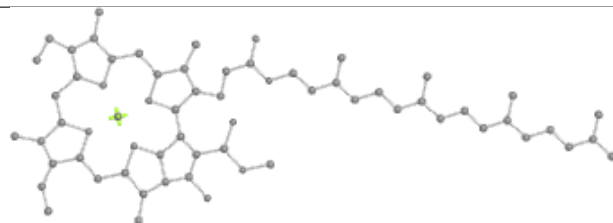
Bond lengths



Bond angles

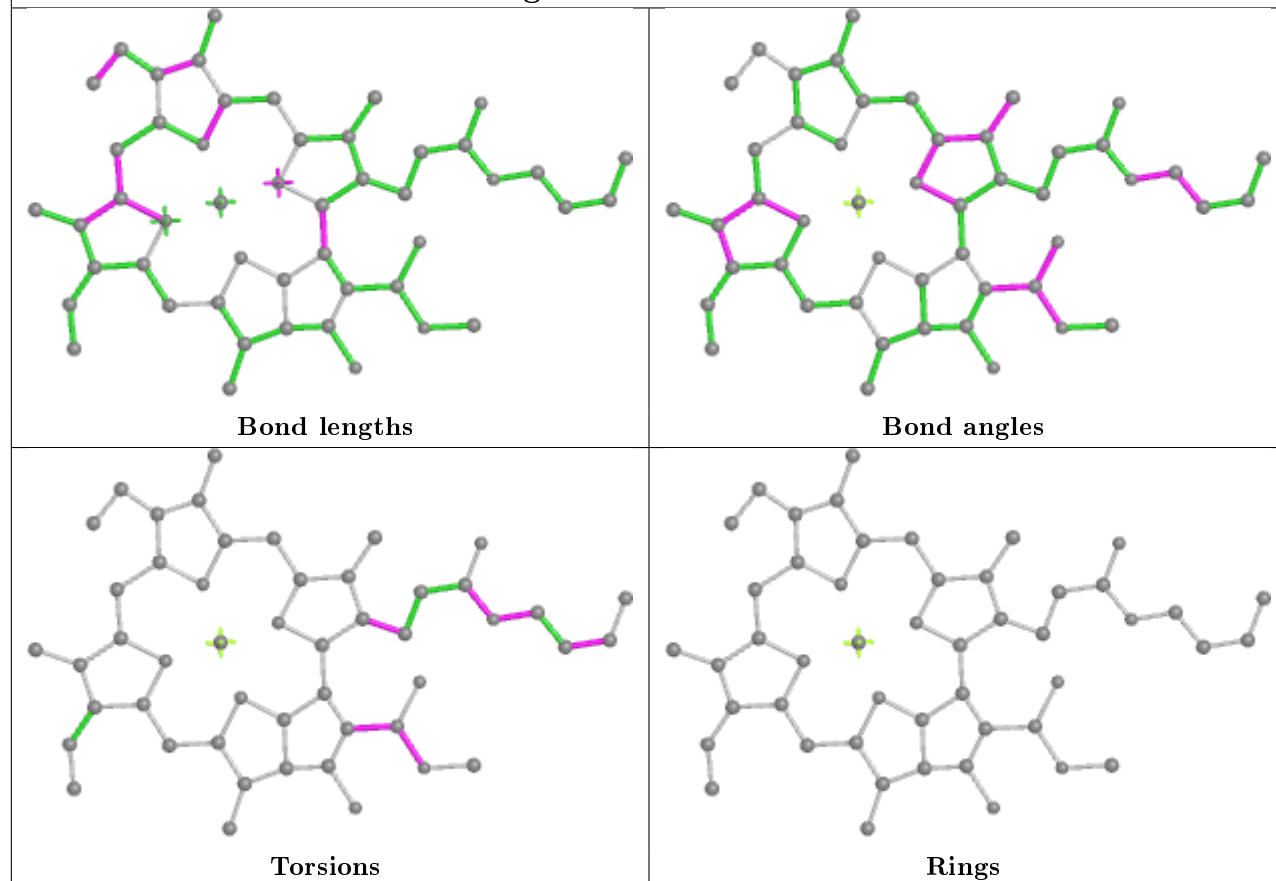


Torsions

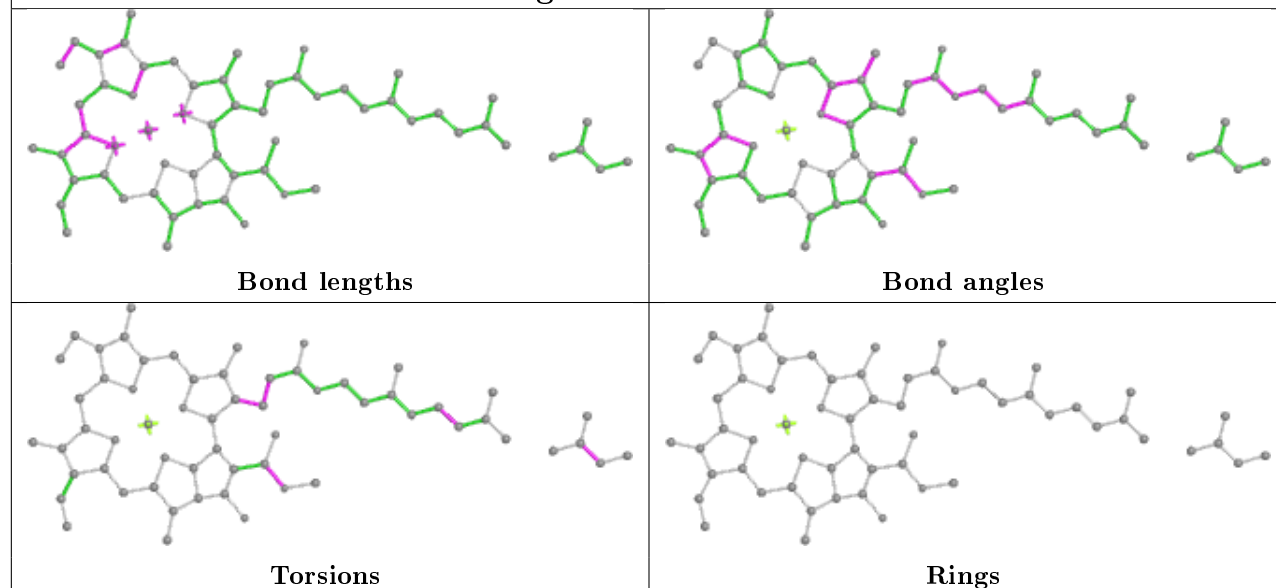


Rings

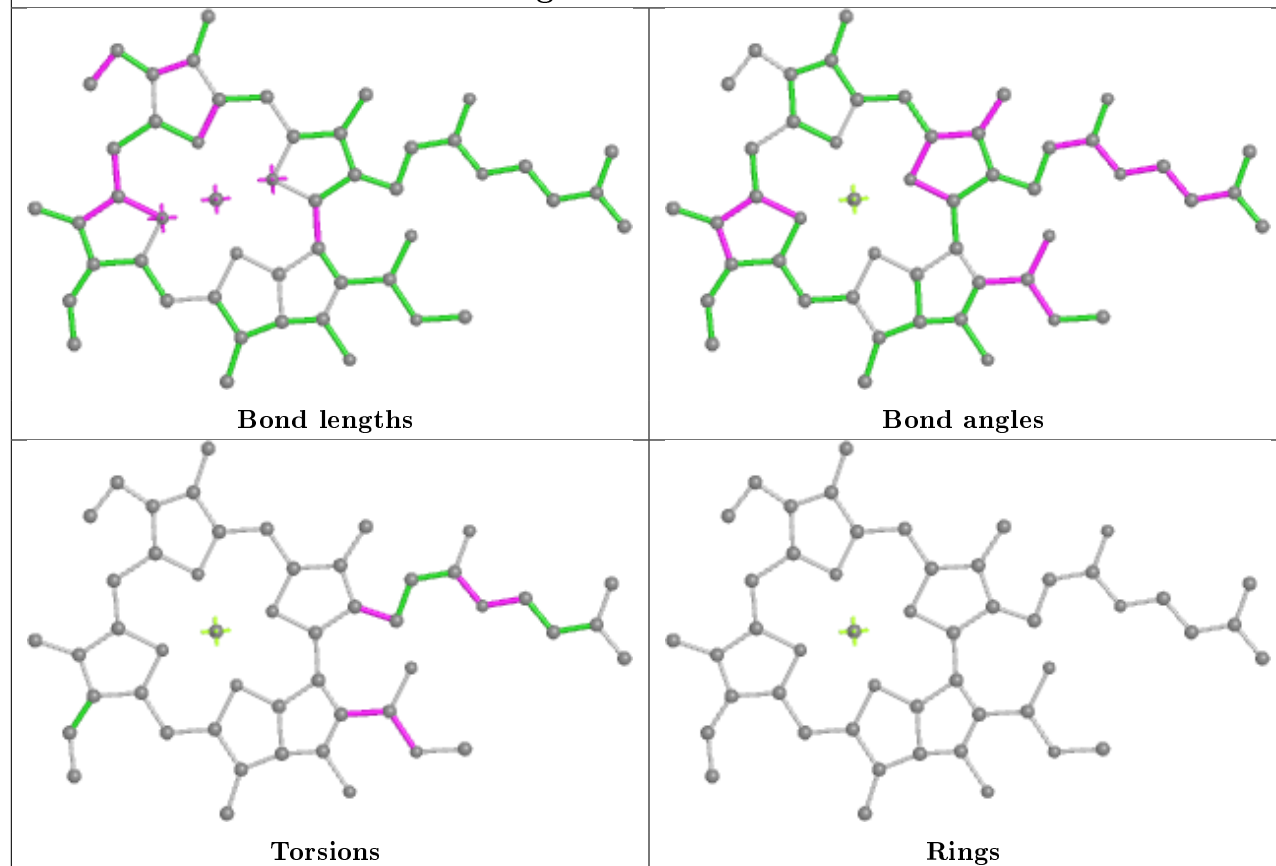
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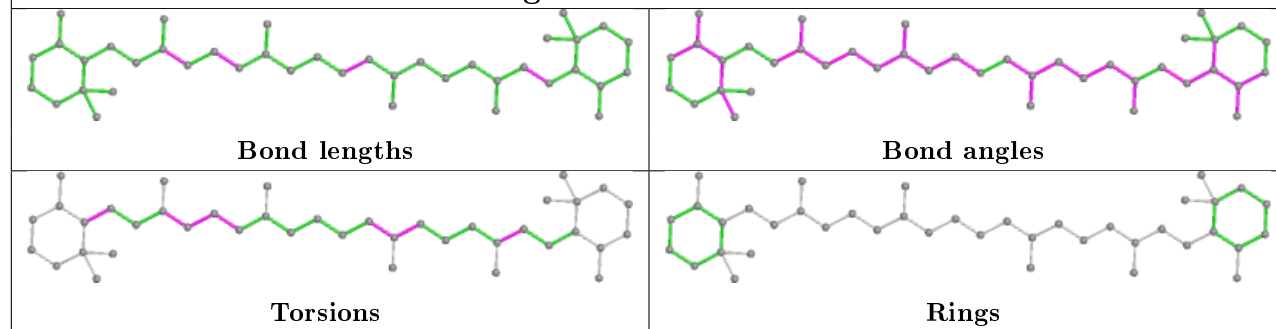
Ligand CLA 1 612



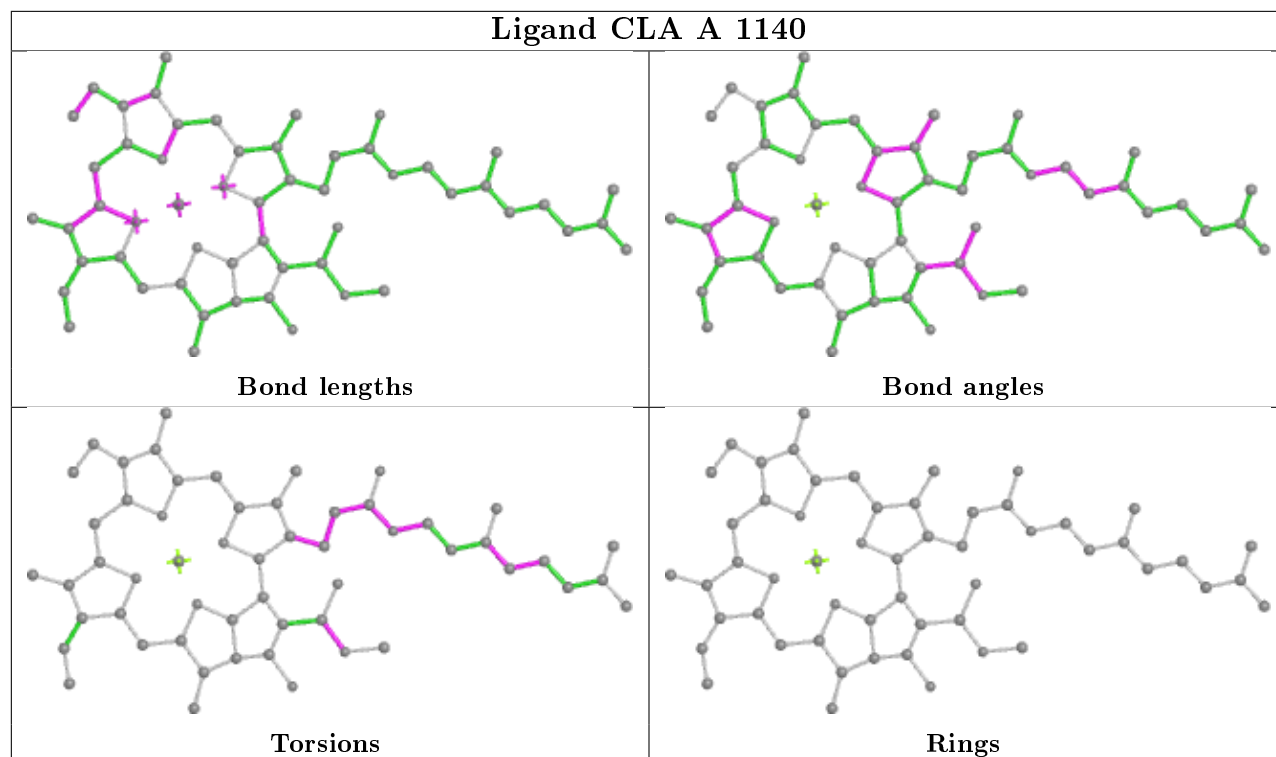
Ligand CLA 2 615



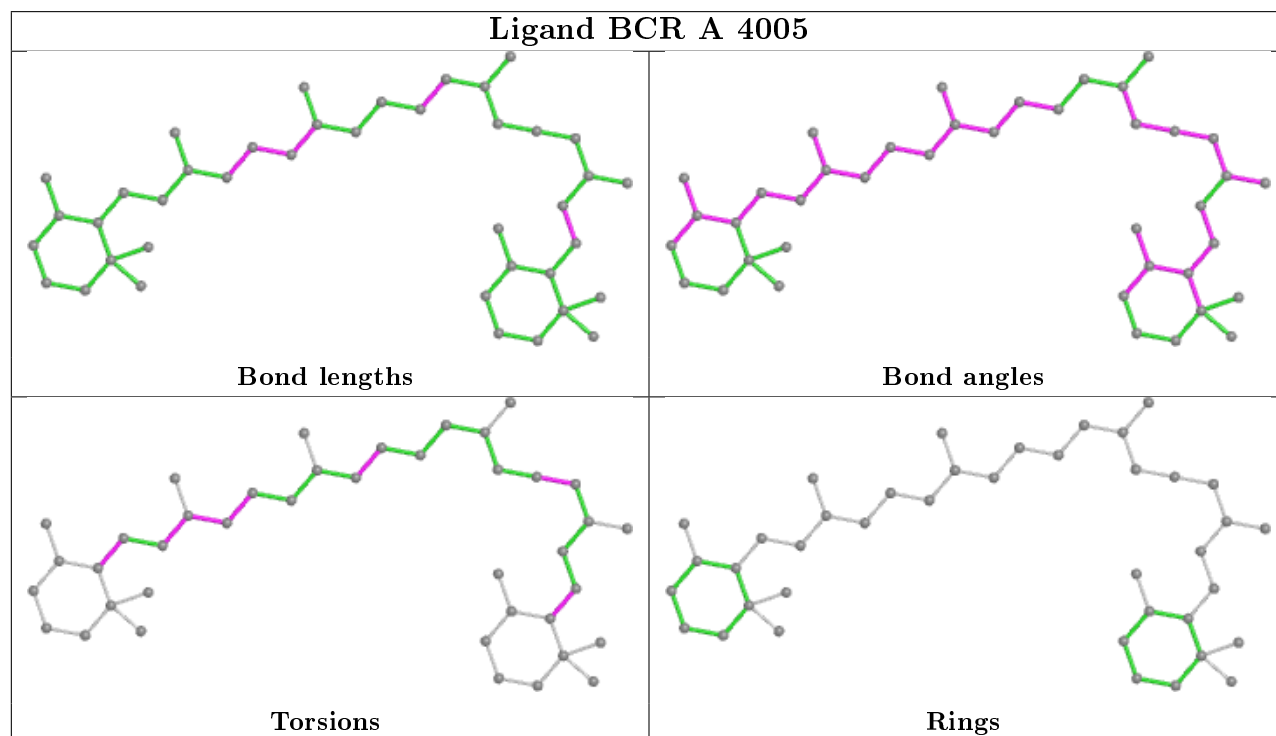
Ligand BCR F 4002



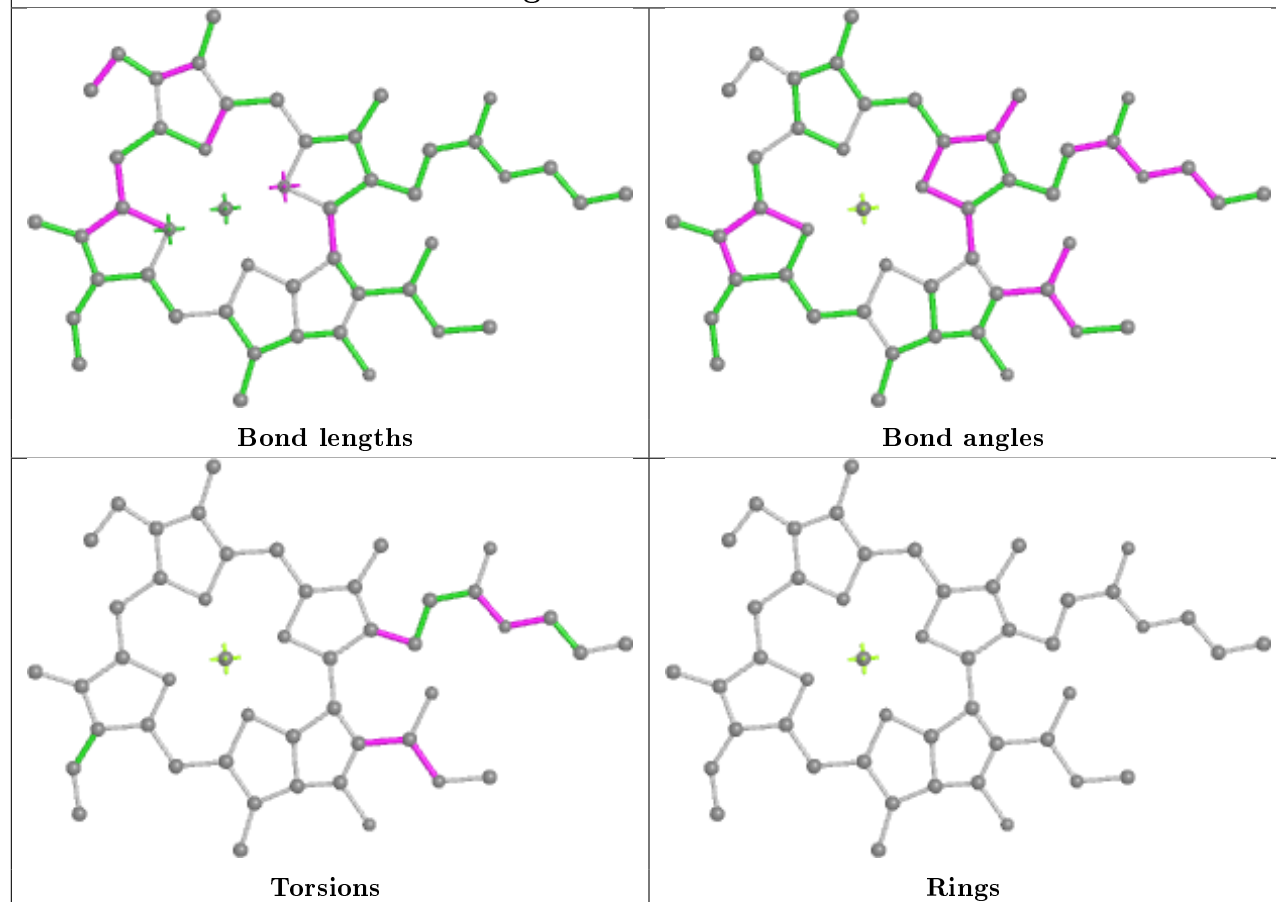
Ligand CLA A 1140



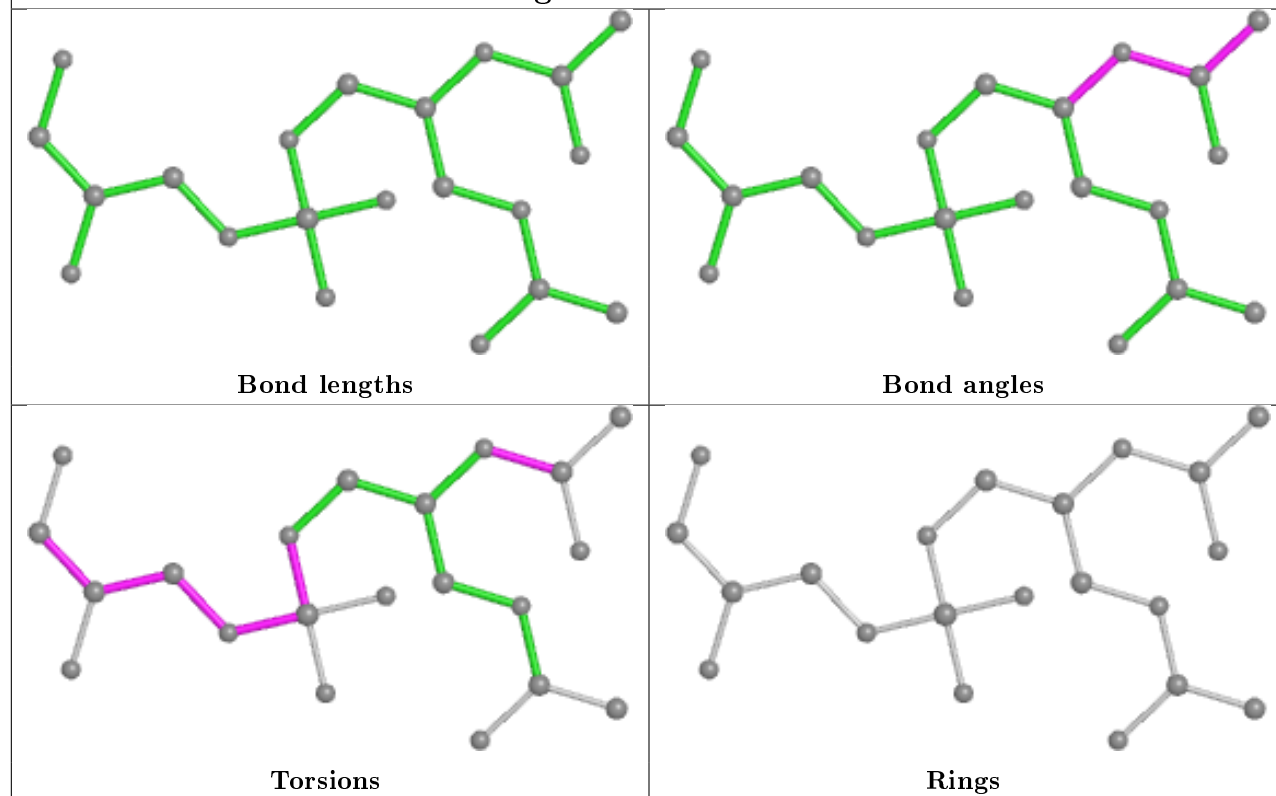
Ligand BCR A 4005



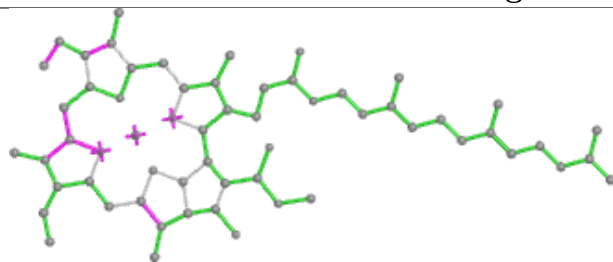
Ligand CLA A 1123



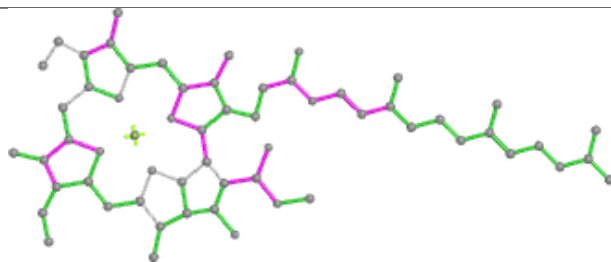
Ligand LHG 2 801



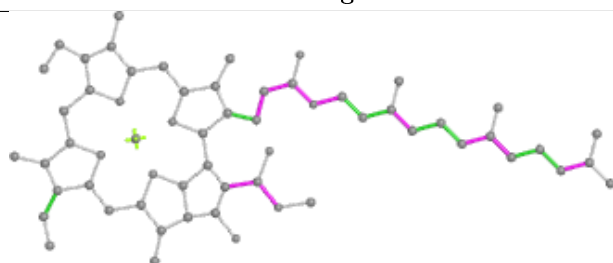
Ligand CLA B 1023



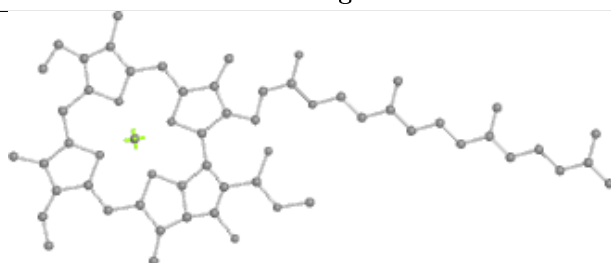
Bond lengths



Bond angles

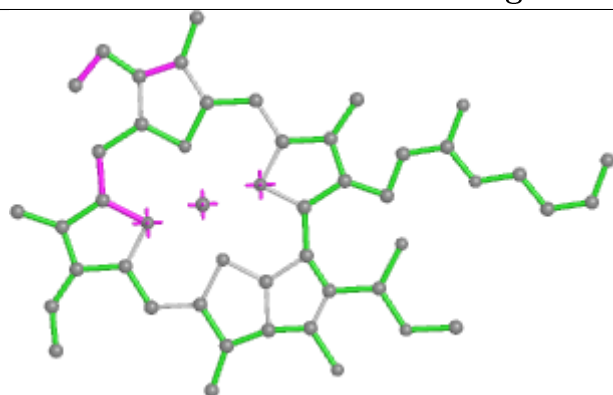


Torsions

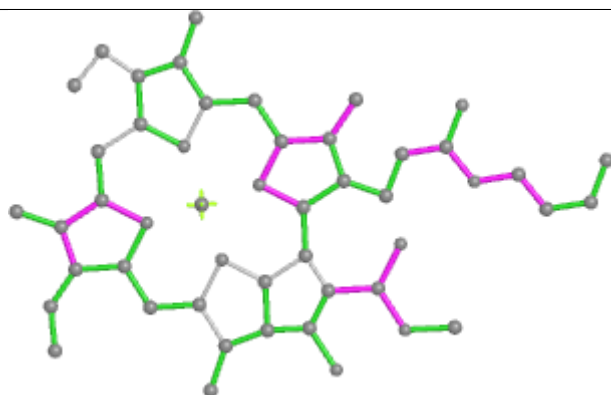


Rings

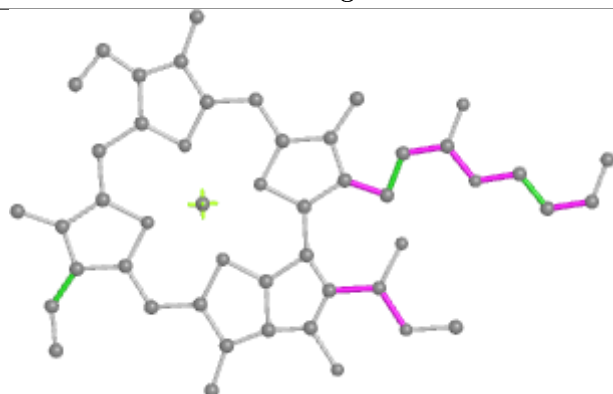
Ligand CLA B 1210



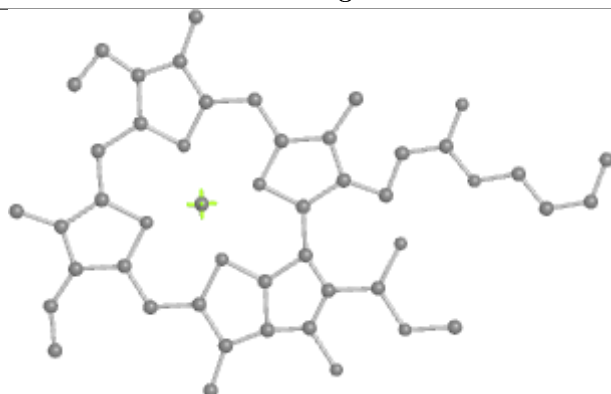
Bond lengths



Bond angles

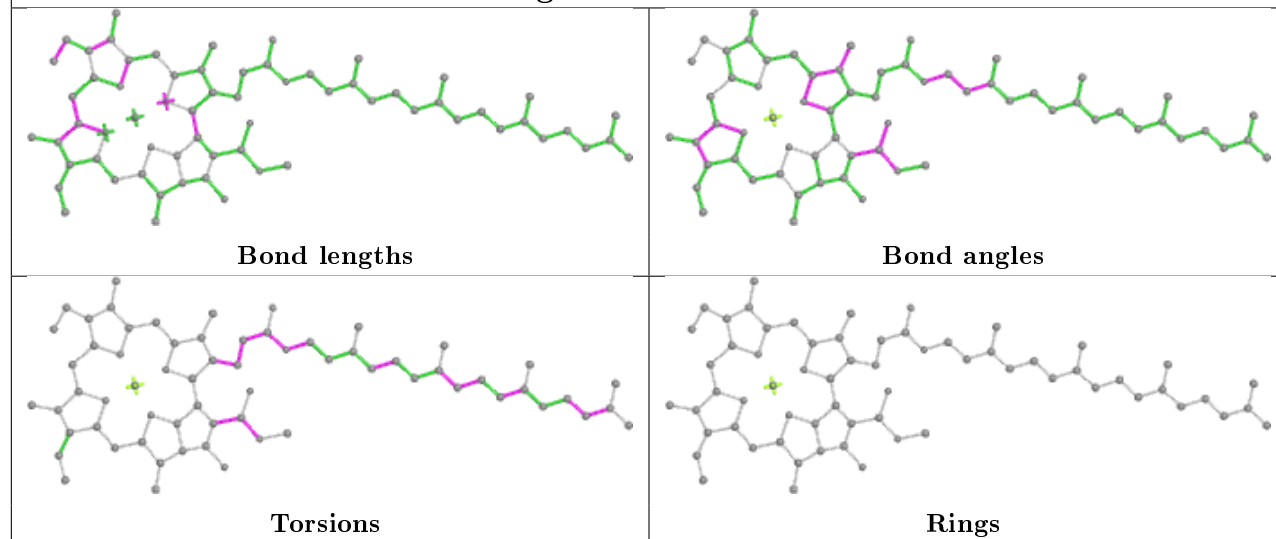


Torsions

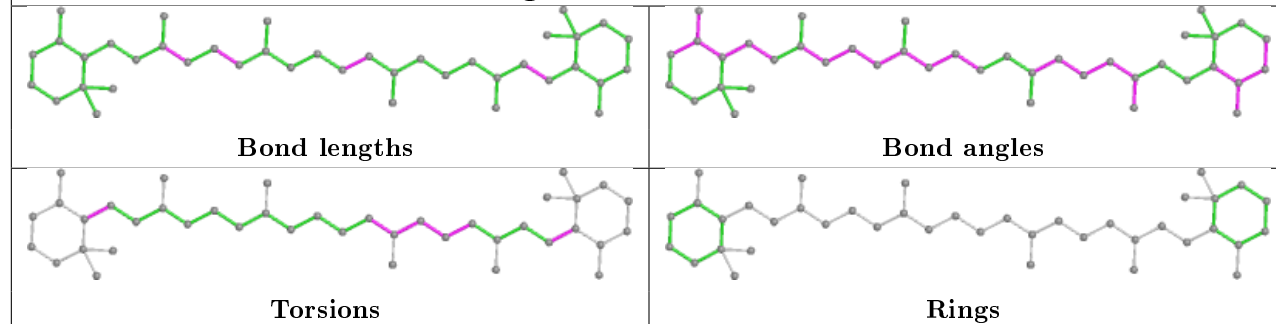


Rings

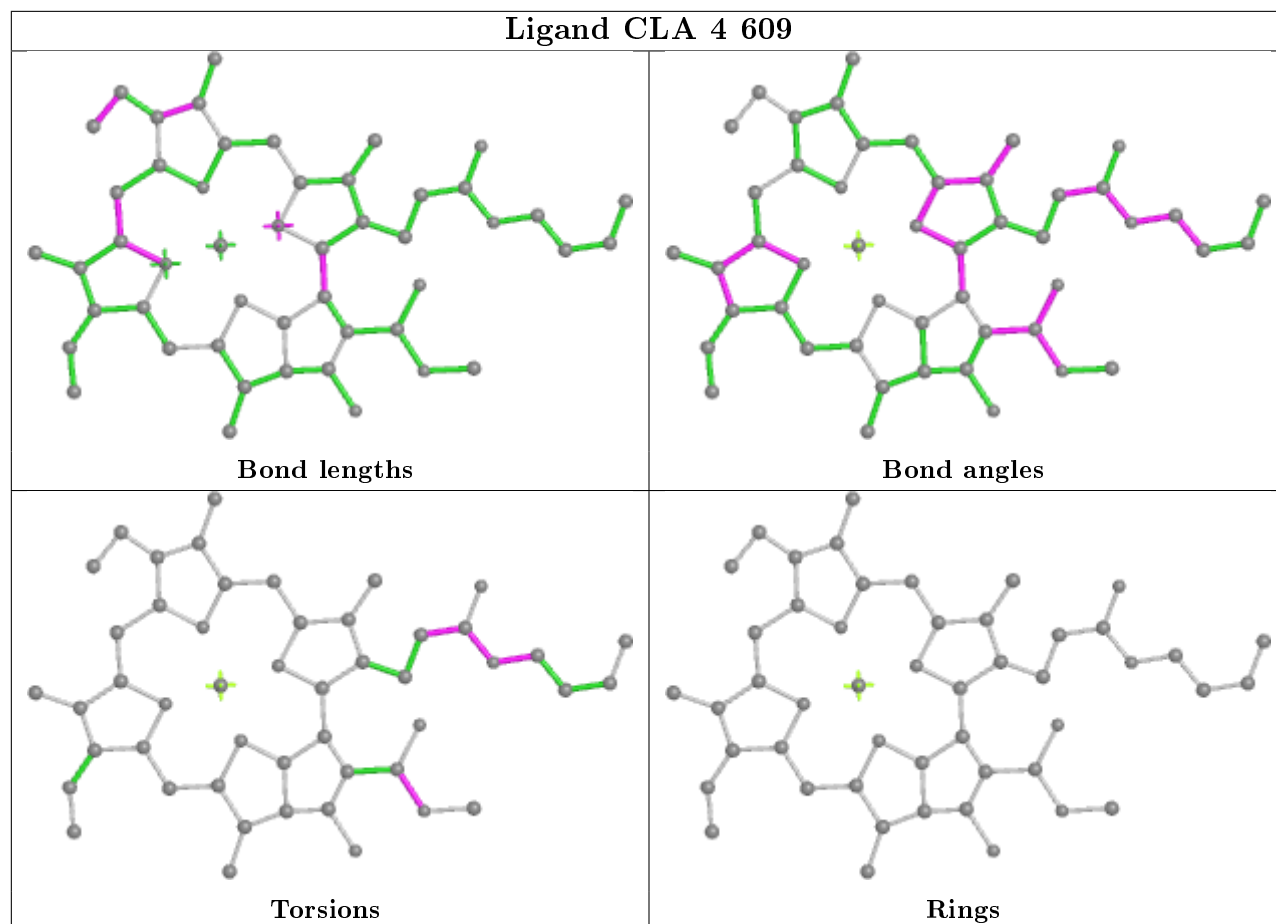
Ligand CLA 1 615

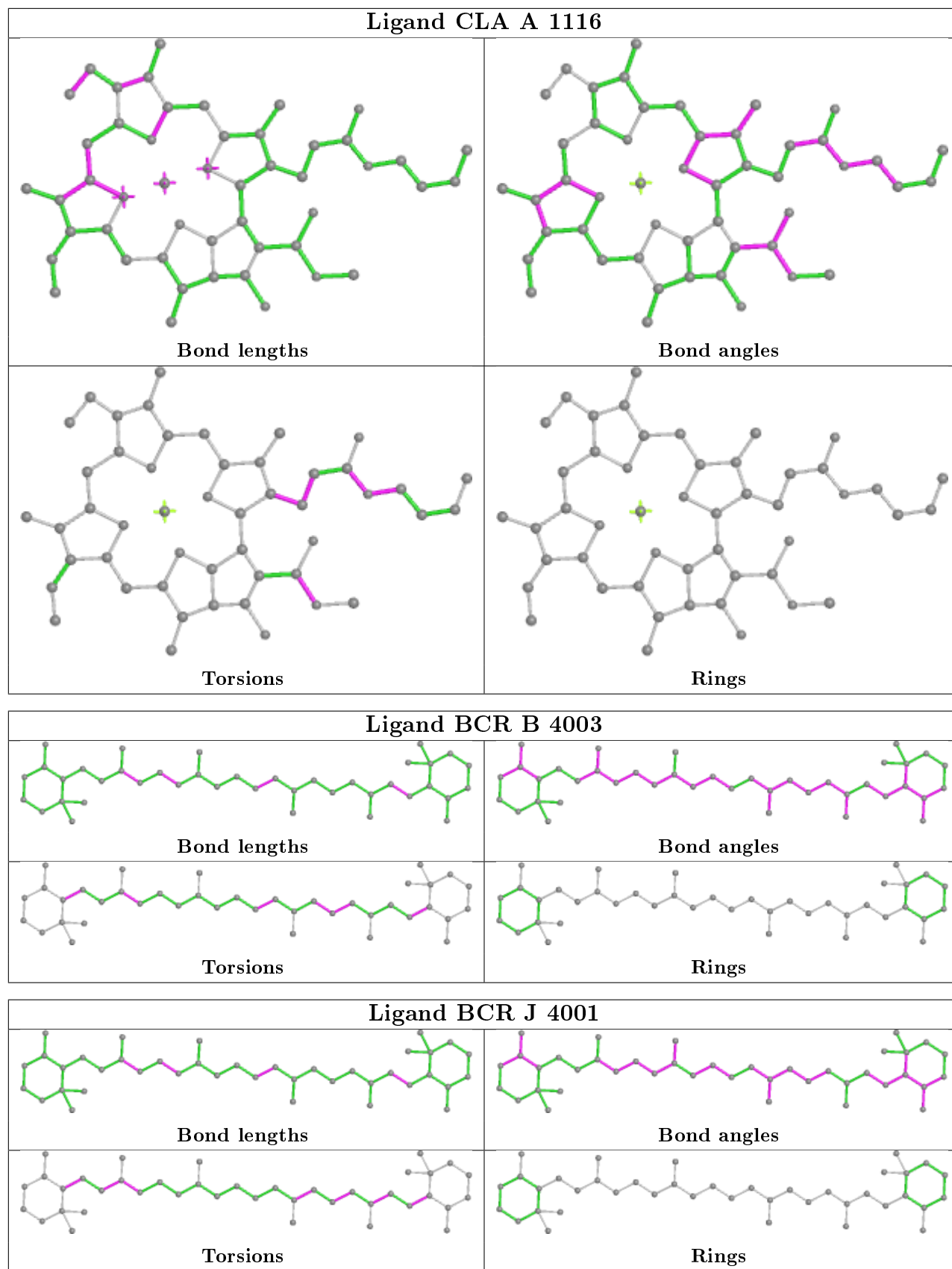


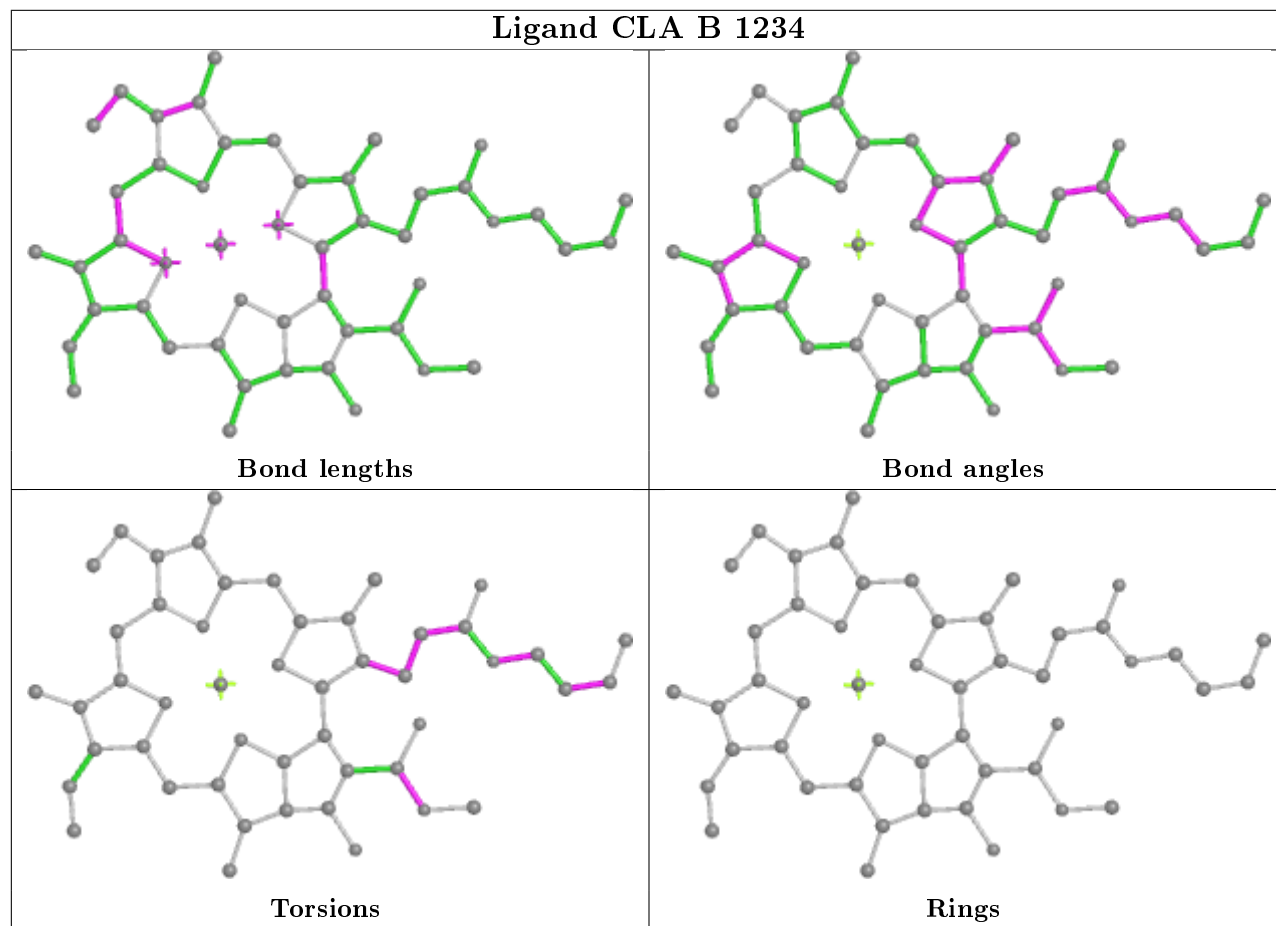
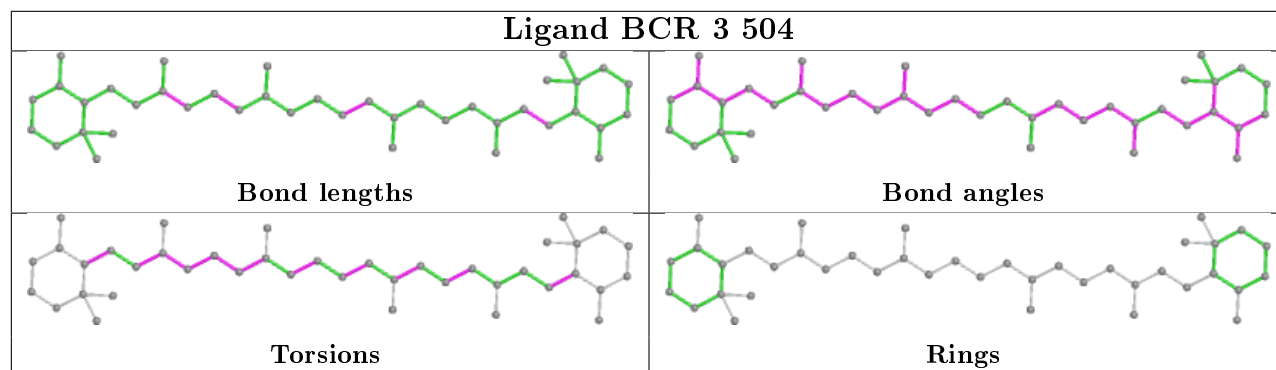
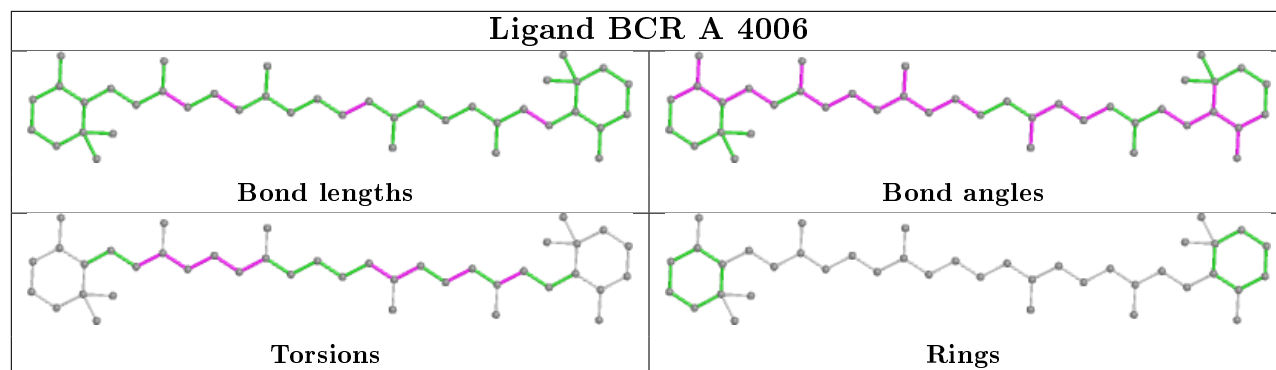
Ligand BCR A 4004

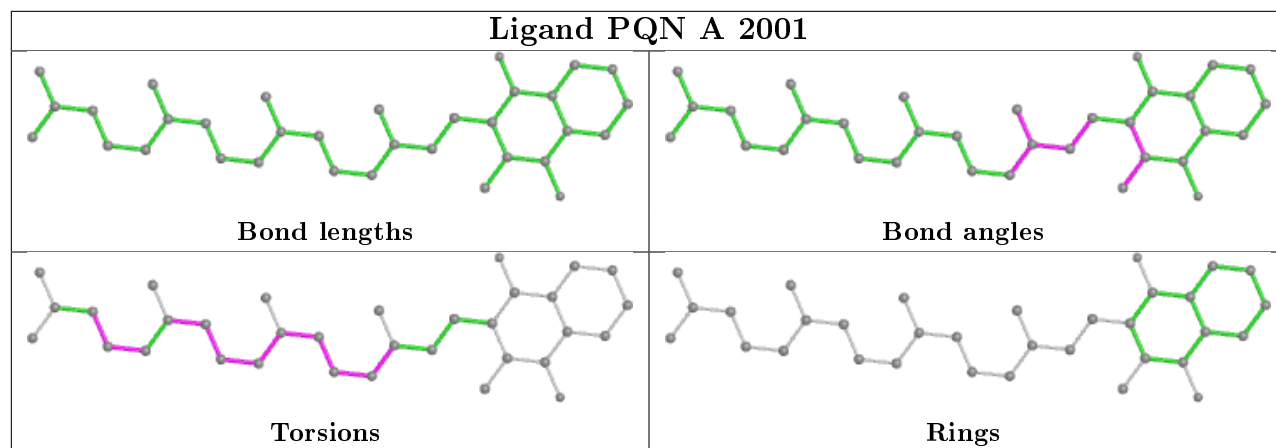
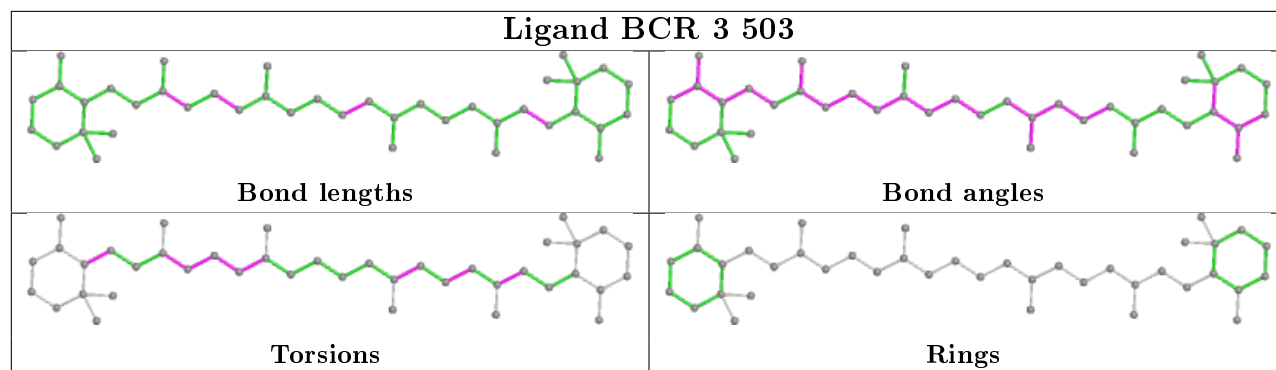


Ligand CLA 4 609

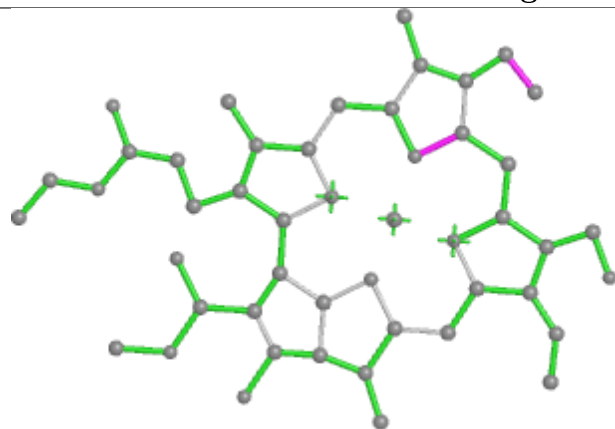




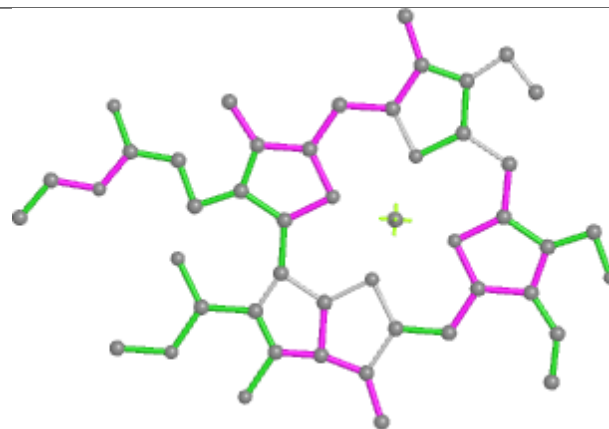




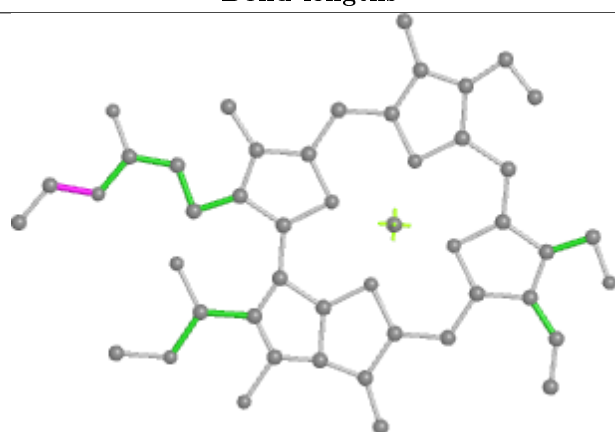
Ligand CHL 2 611



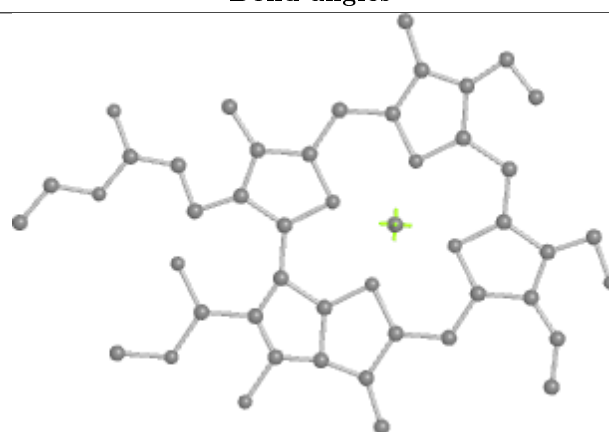
Bond lengths



Bond angles

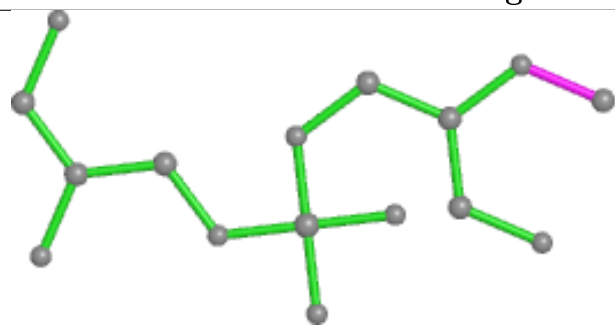


Torsions

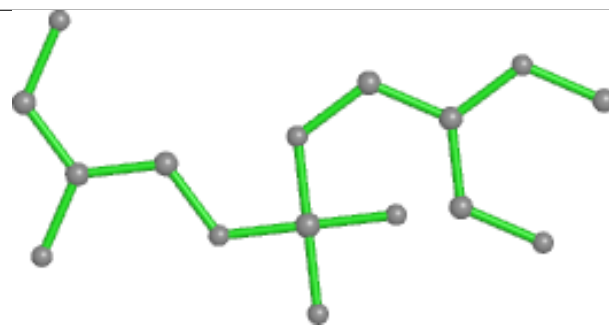


Rings

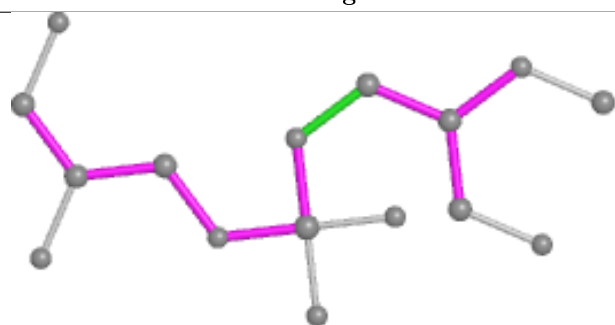
Ligand LHG A 5001



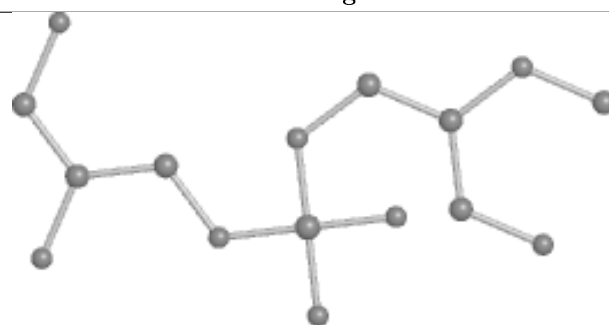
Bond lengths



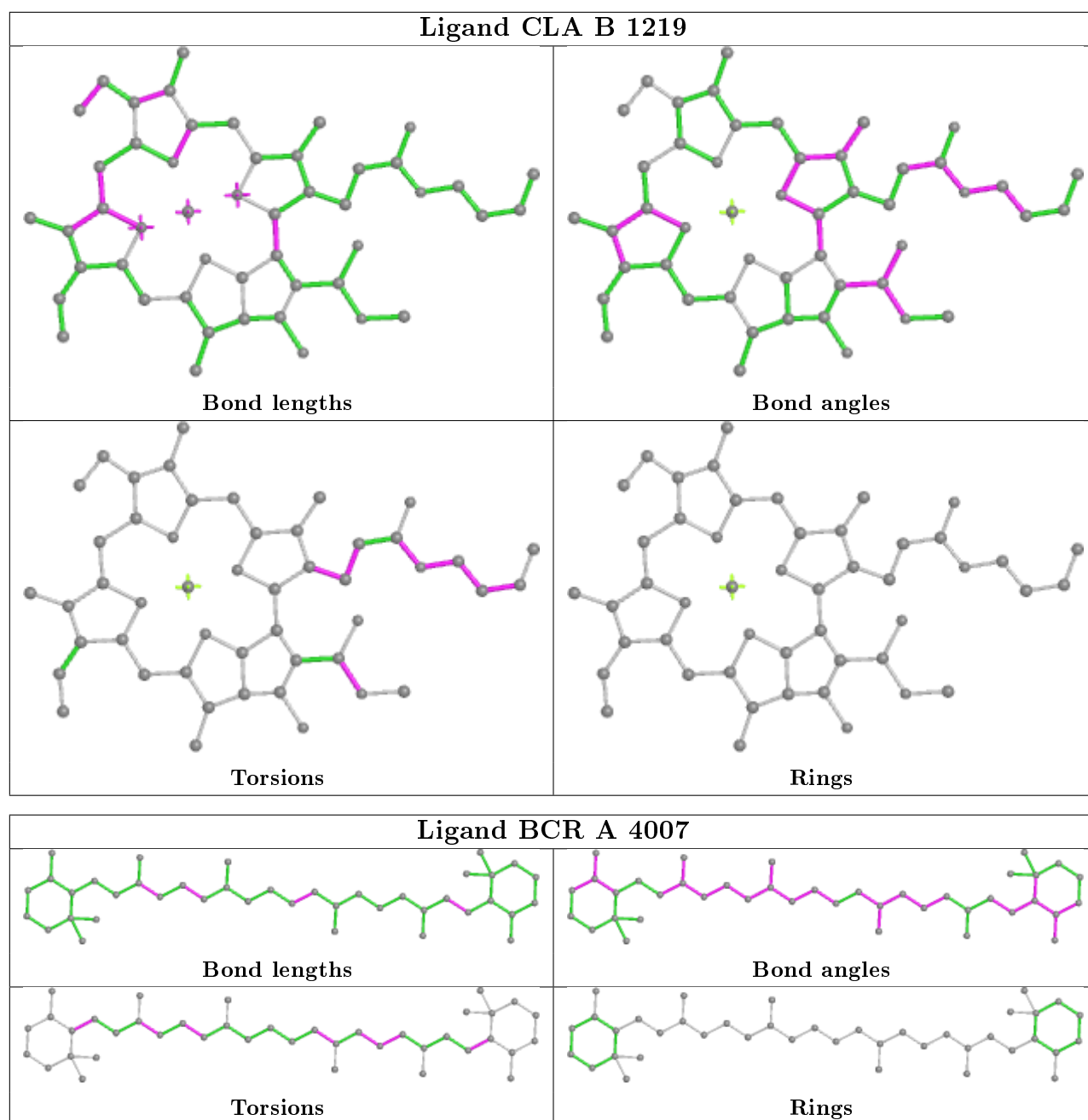
Bond angles

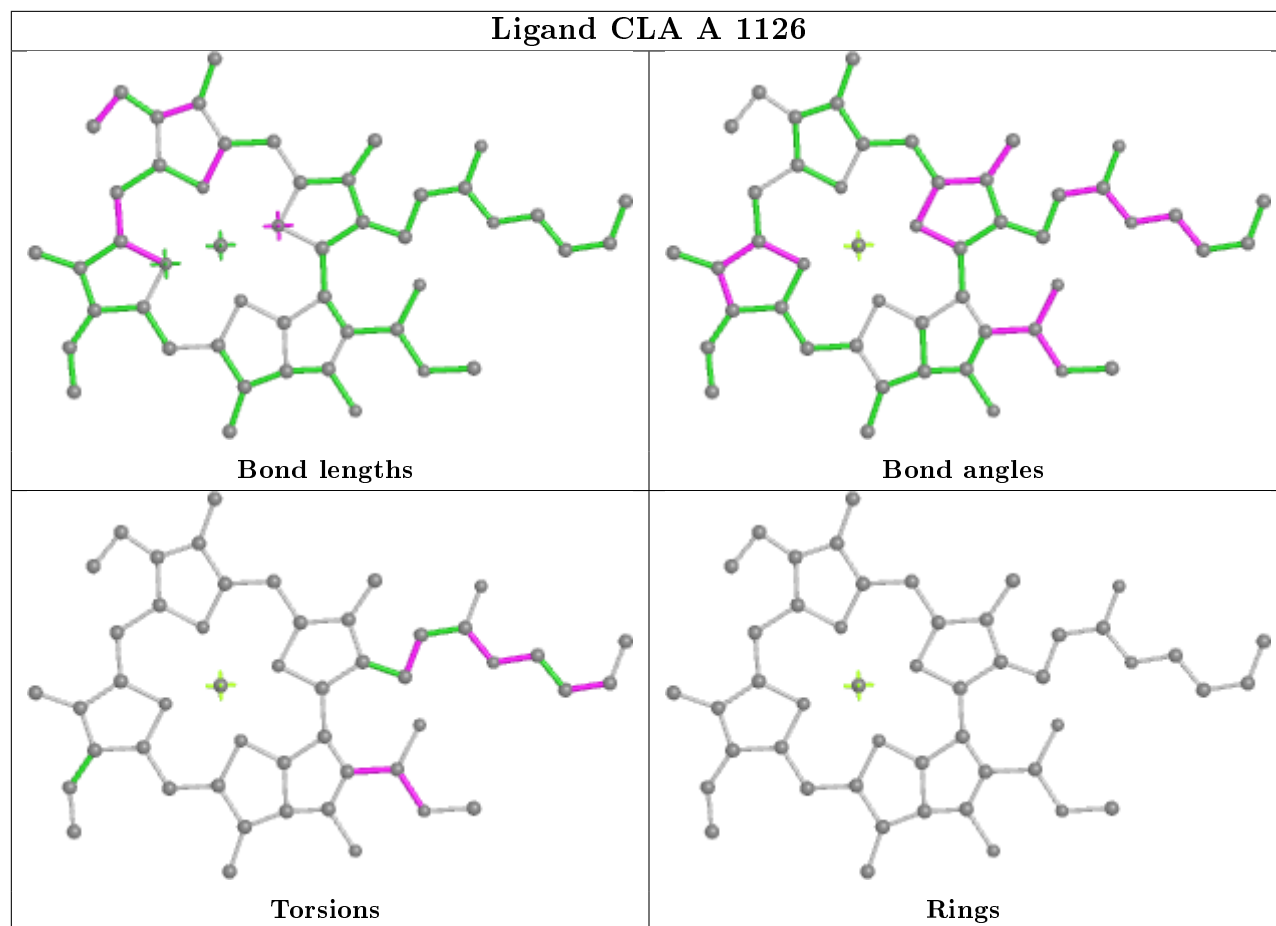


Torsions

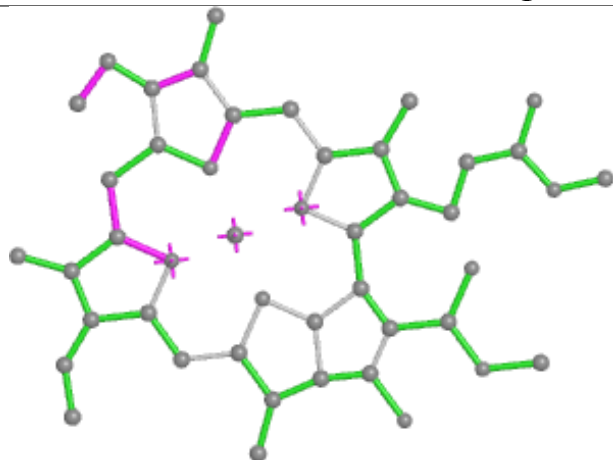


Rings

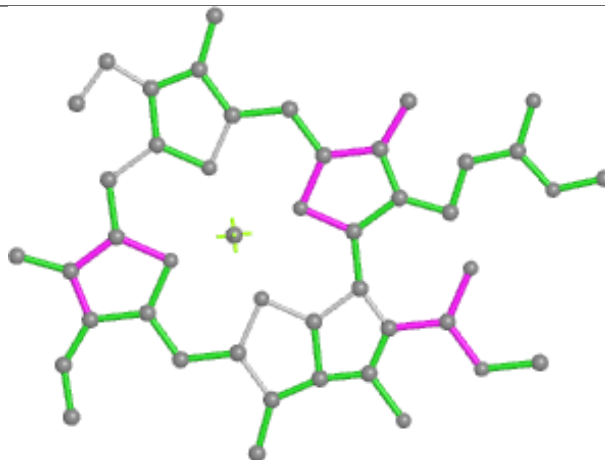




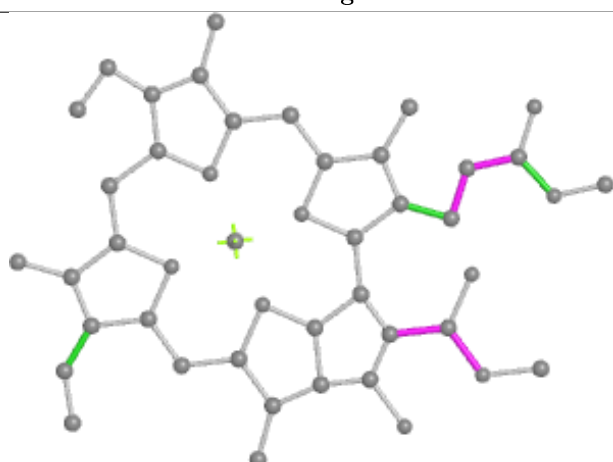
Ligand CLA 2 603



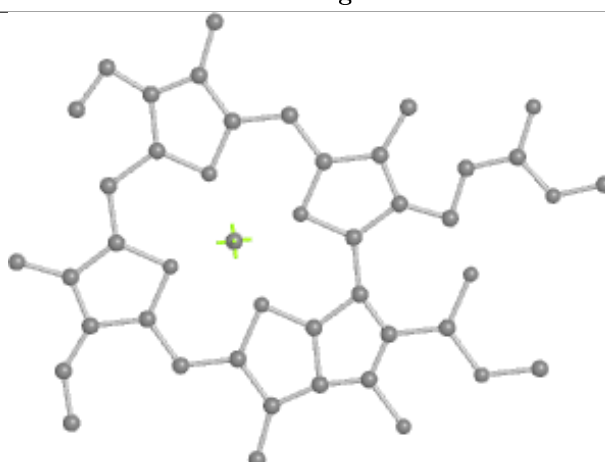
Bond lengths



Bond angles

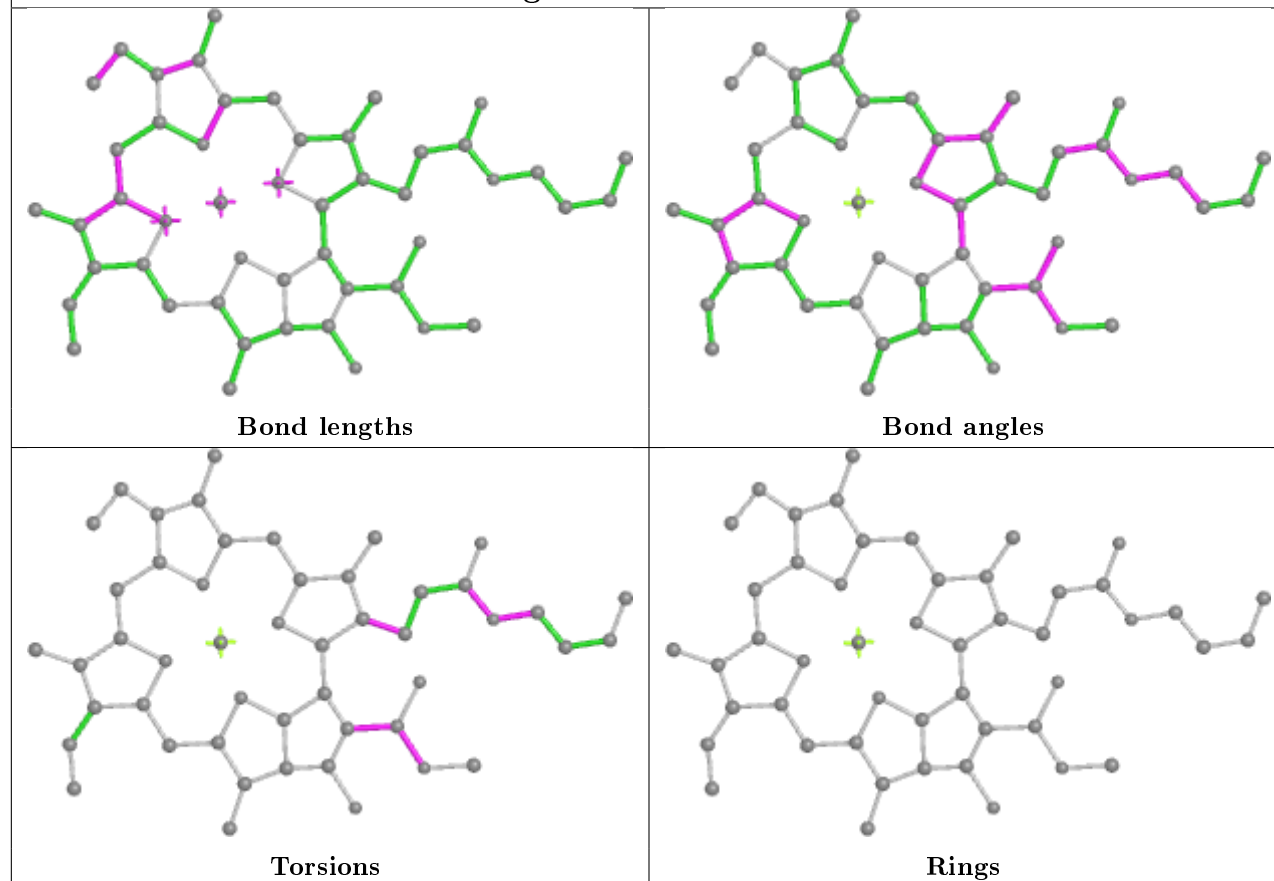


Torsions

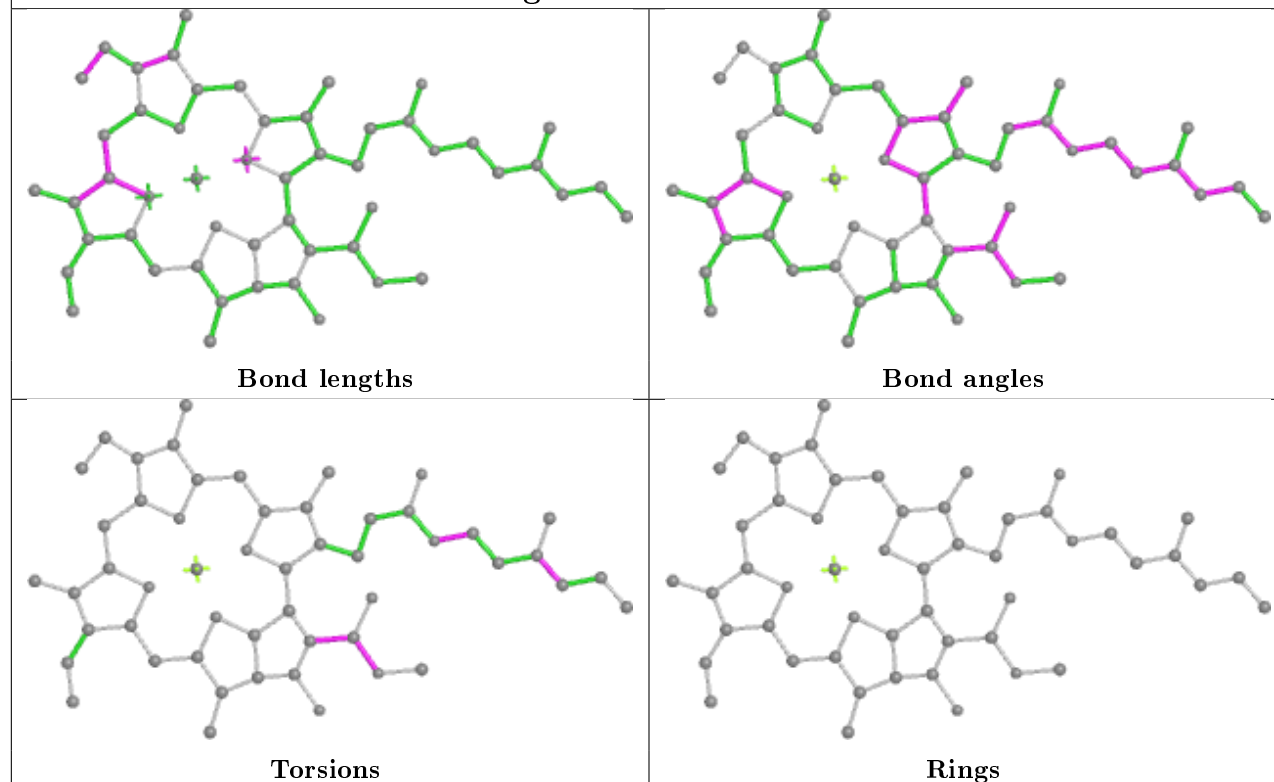


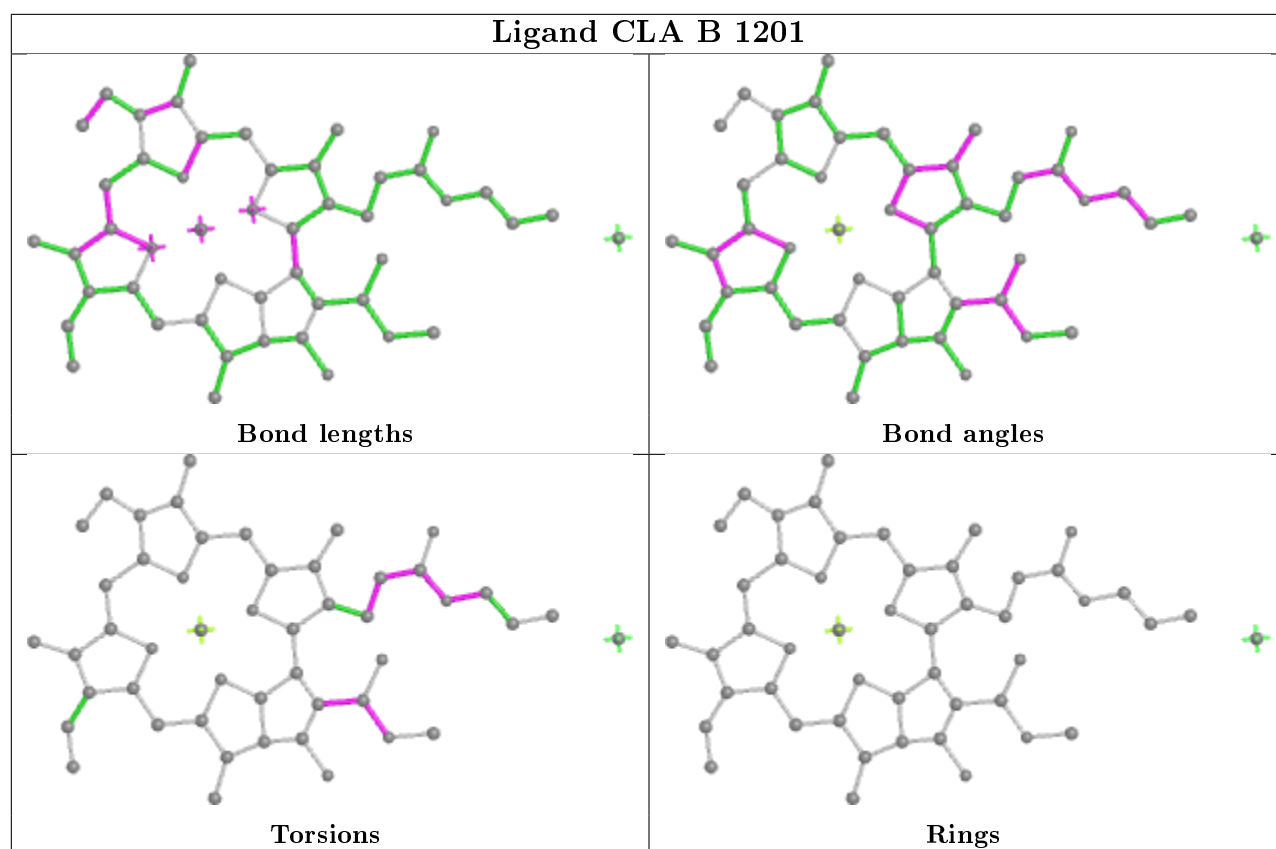
Rings

Ligand CLA A 1112

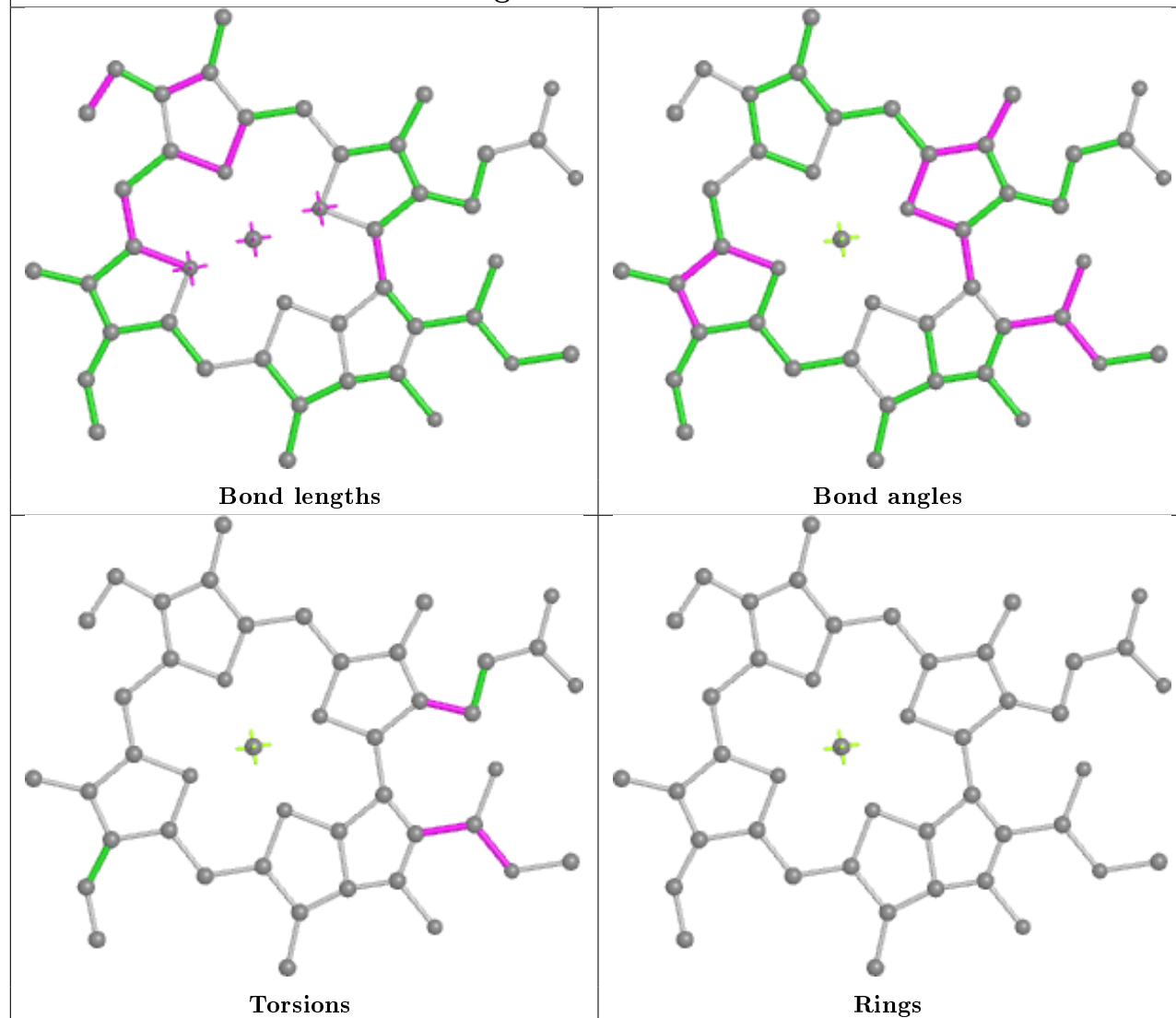


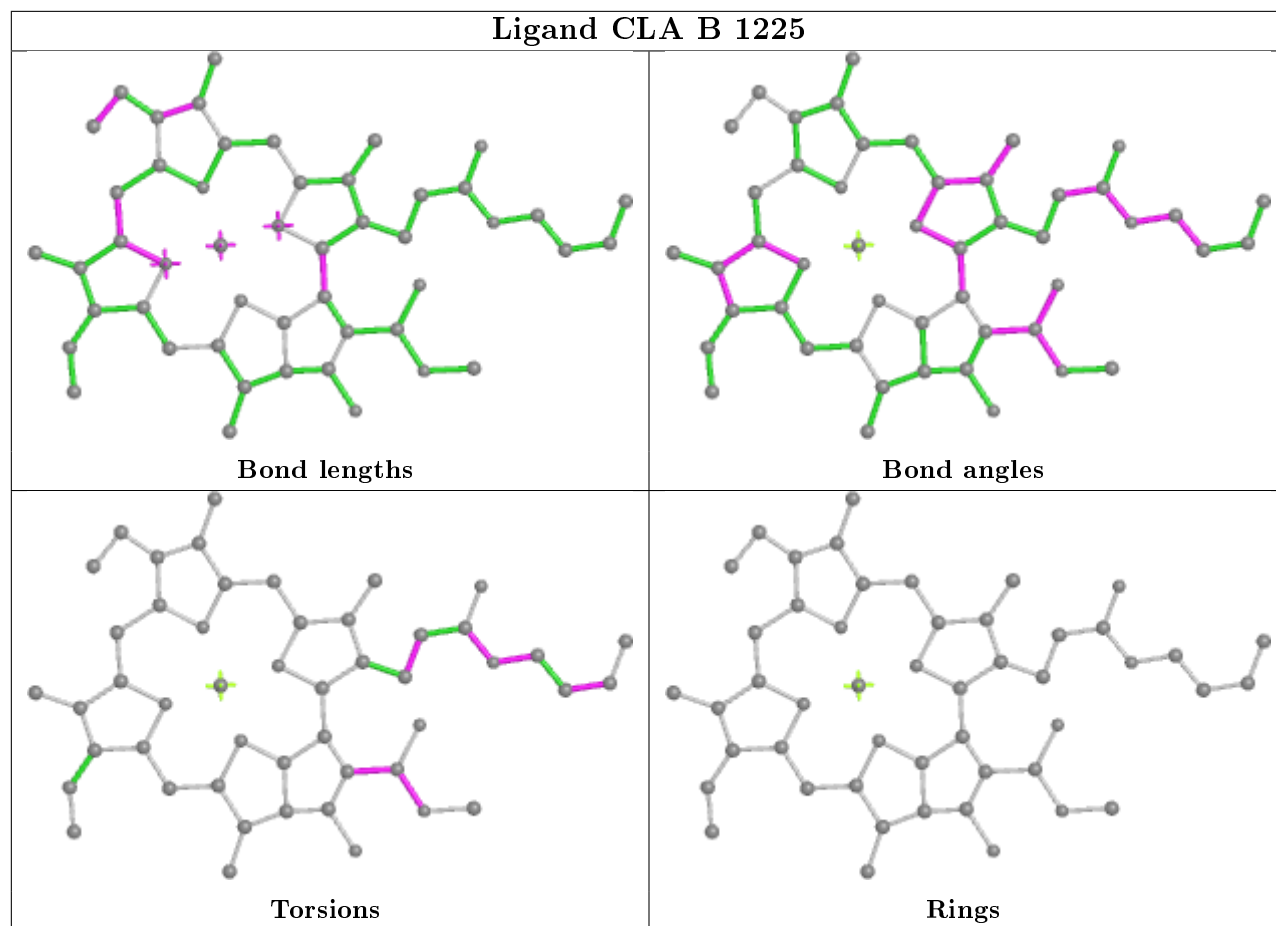
Ligand CLA A 1139

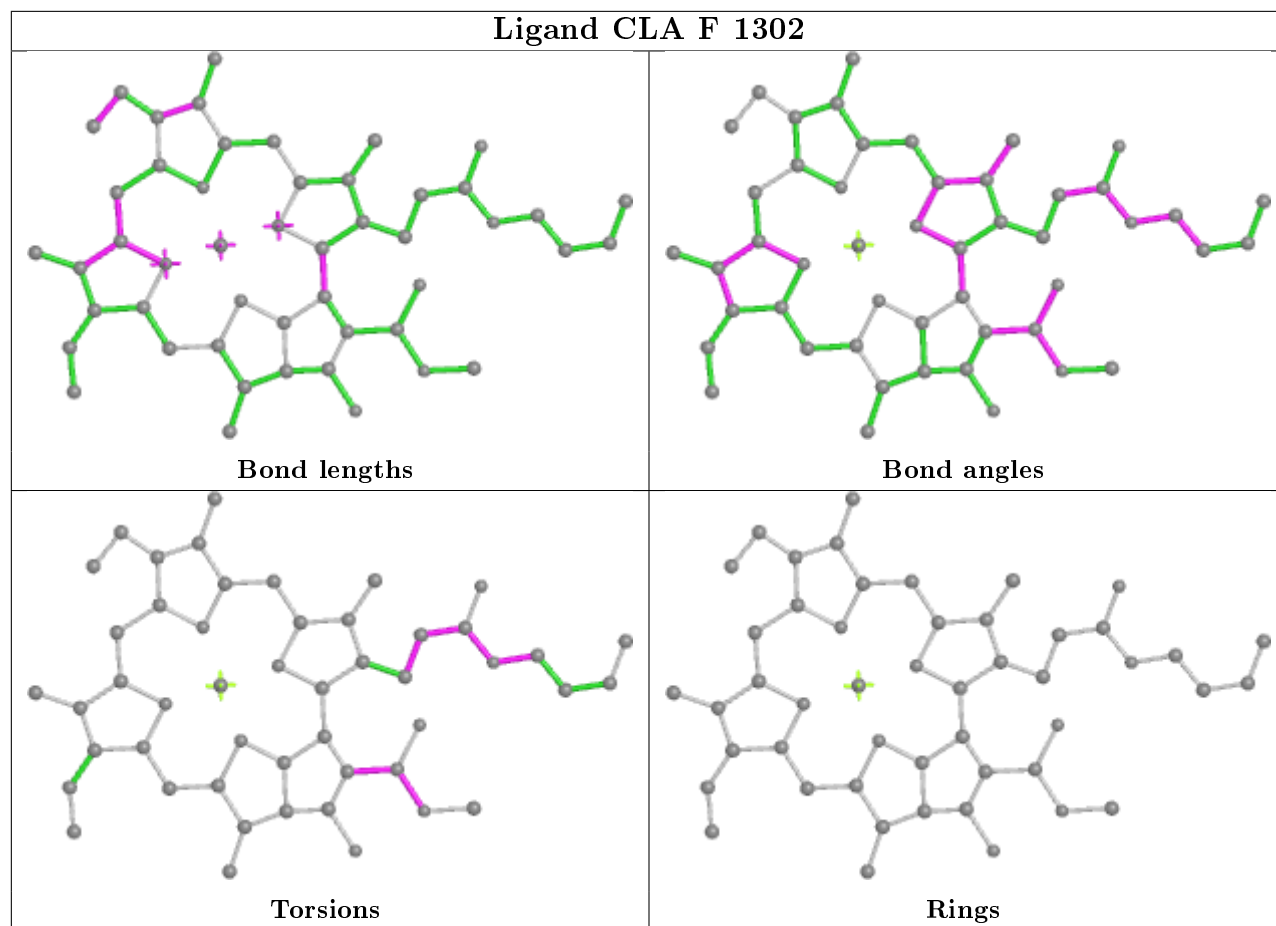




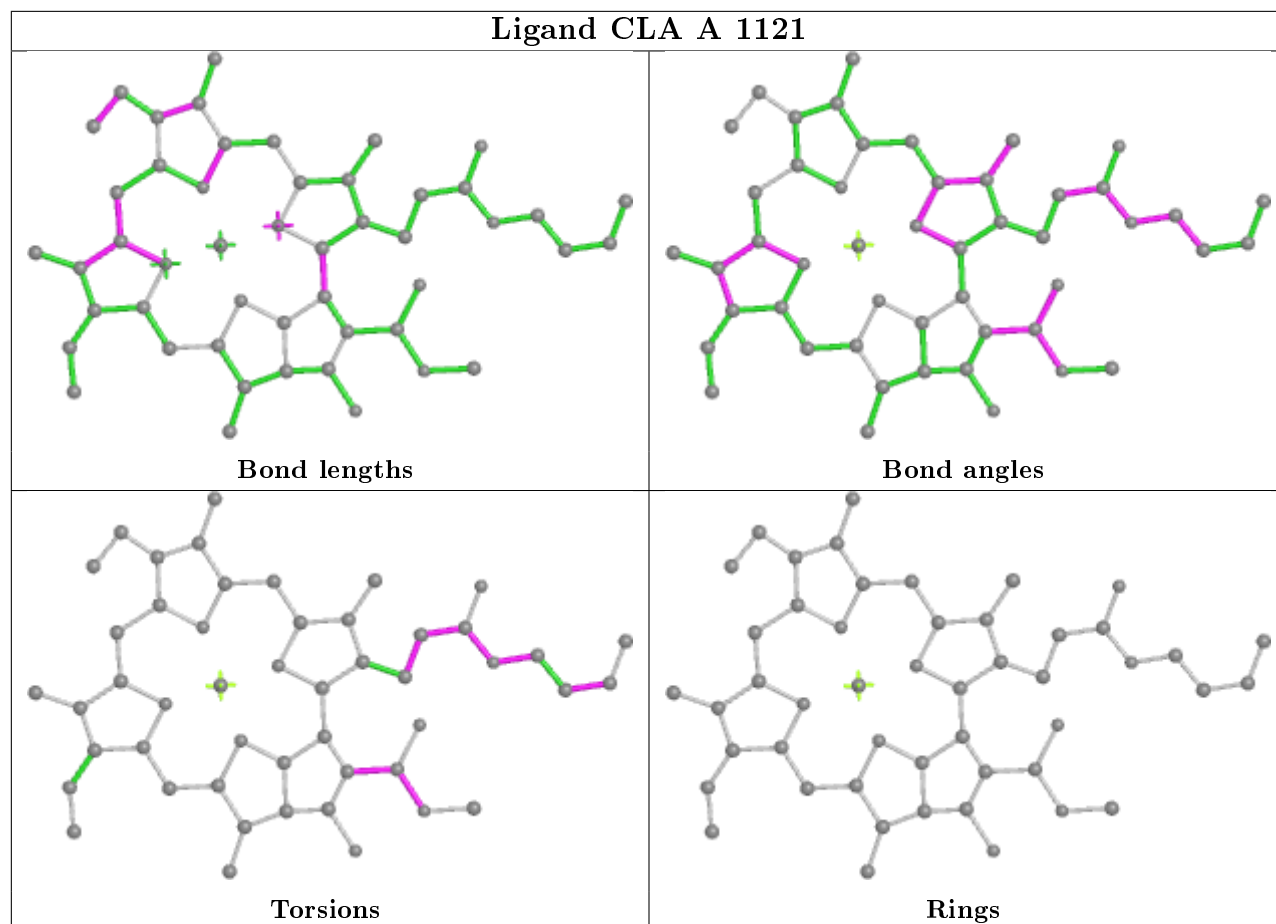
Ligand CLA 1 603



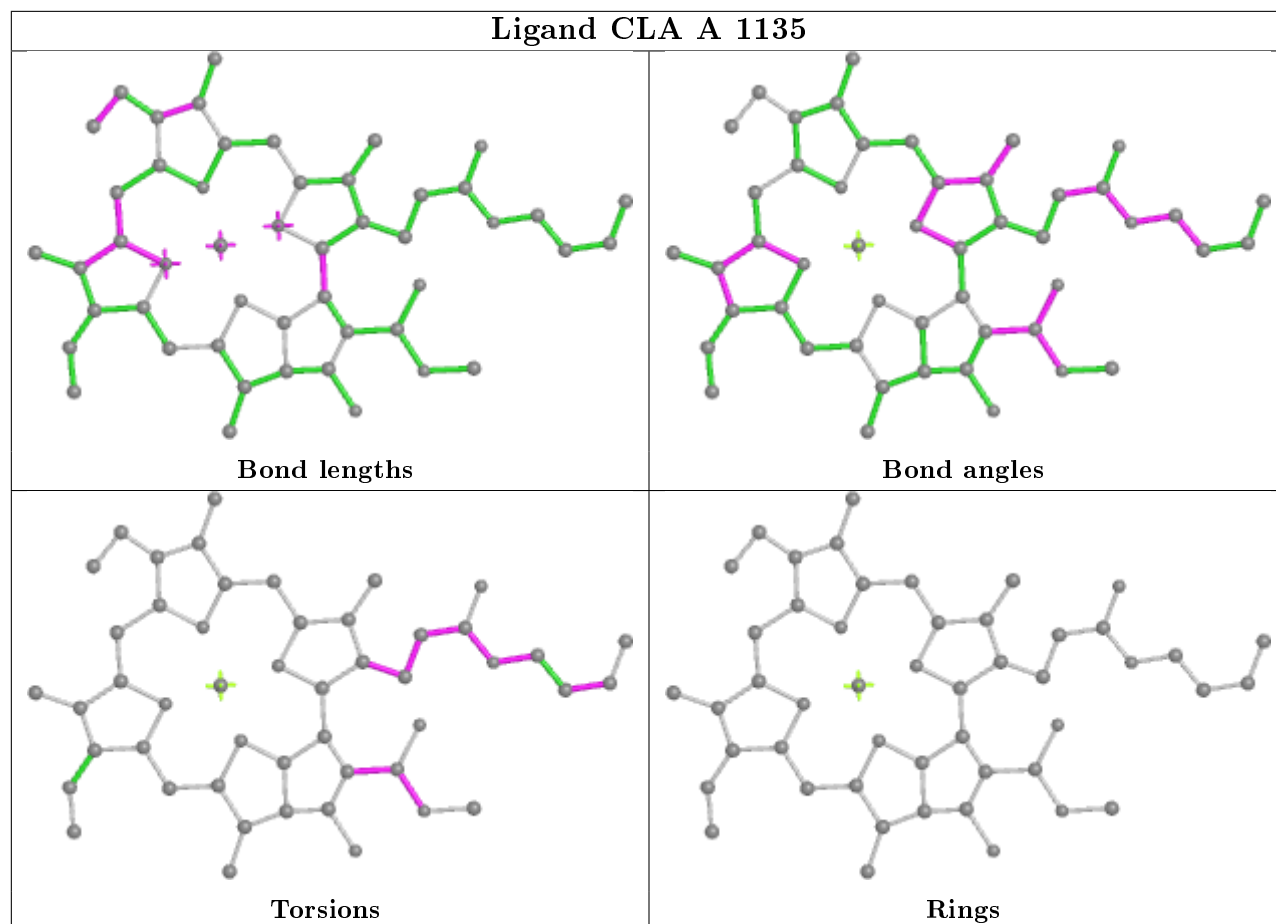




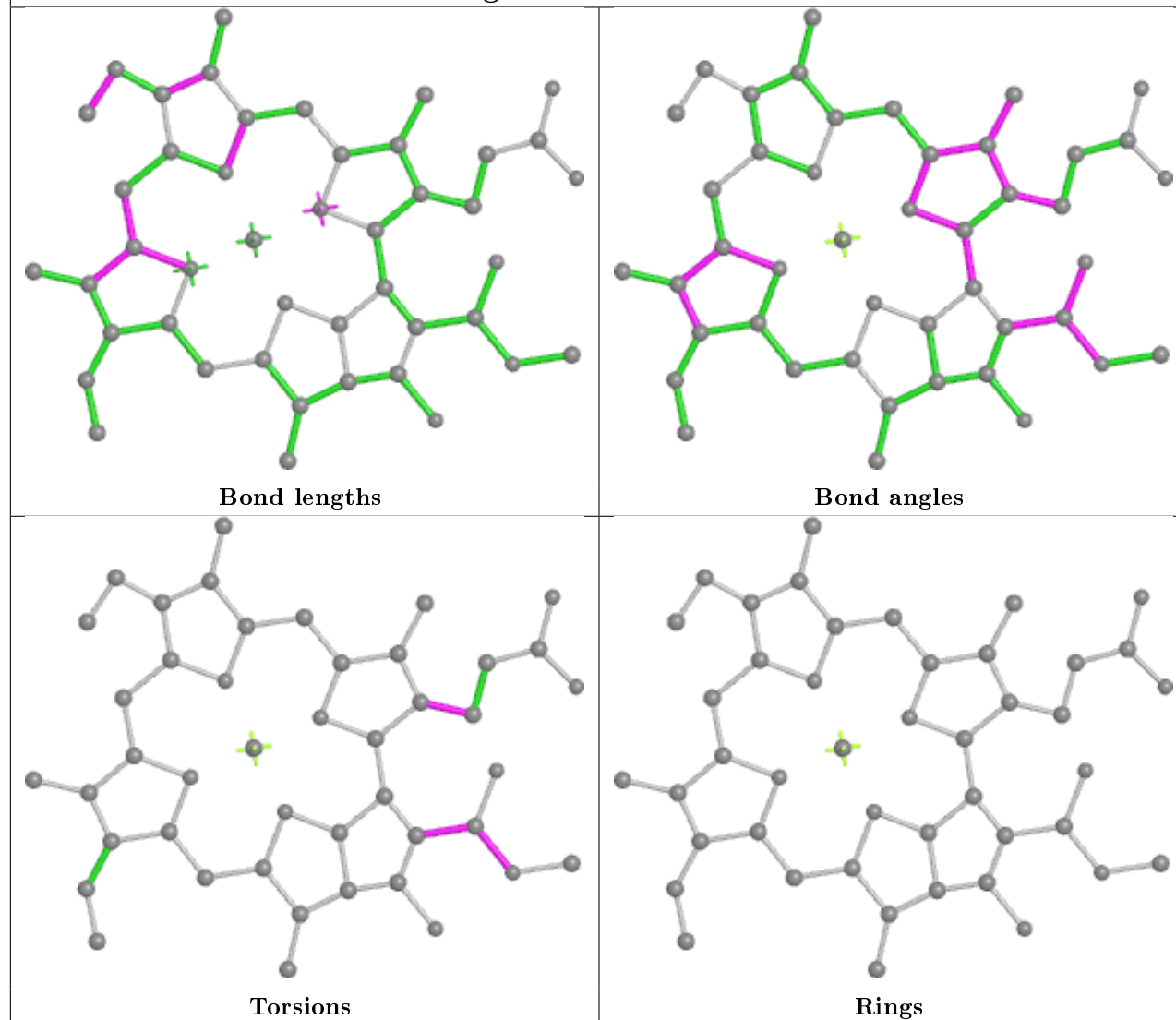
Ligand CLA A 1121



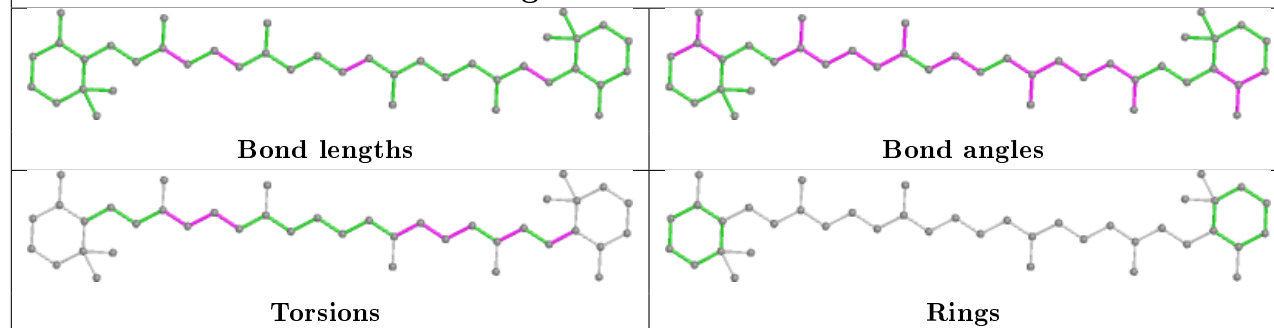
Ligand CLA A 1135



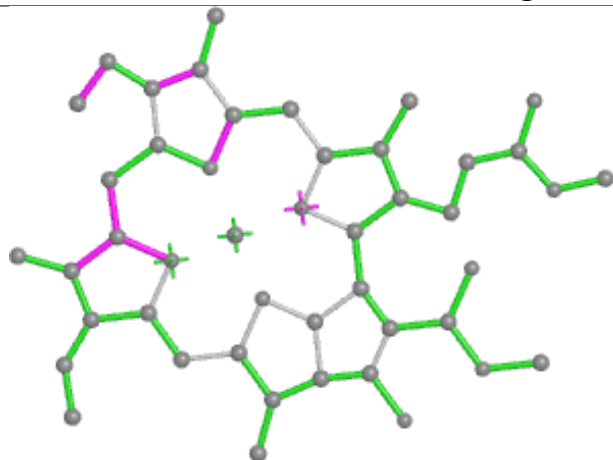
Ligand CLA A 1101



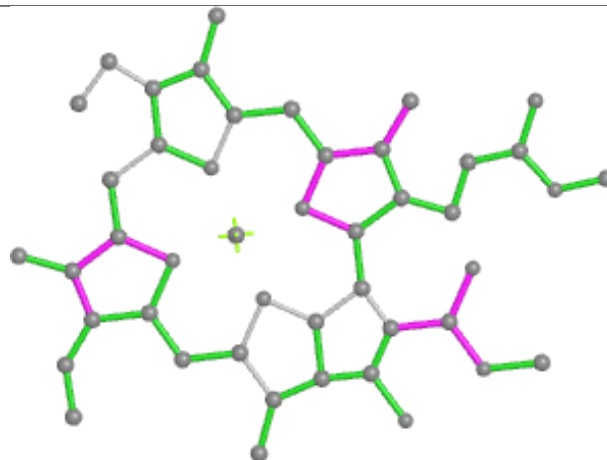
Ligand BCR A 4003



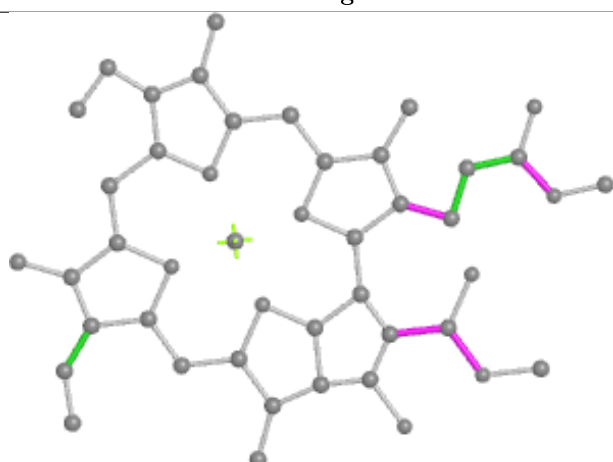
Ligand CLA 1 608



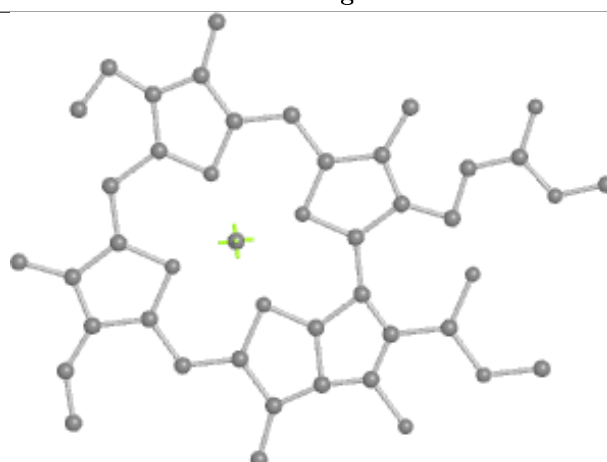
Bond lengths



Bond angles

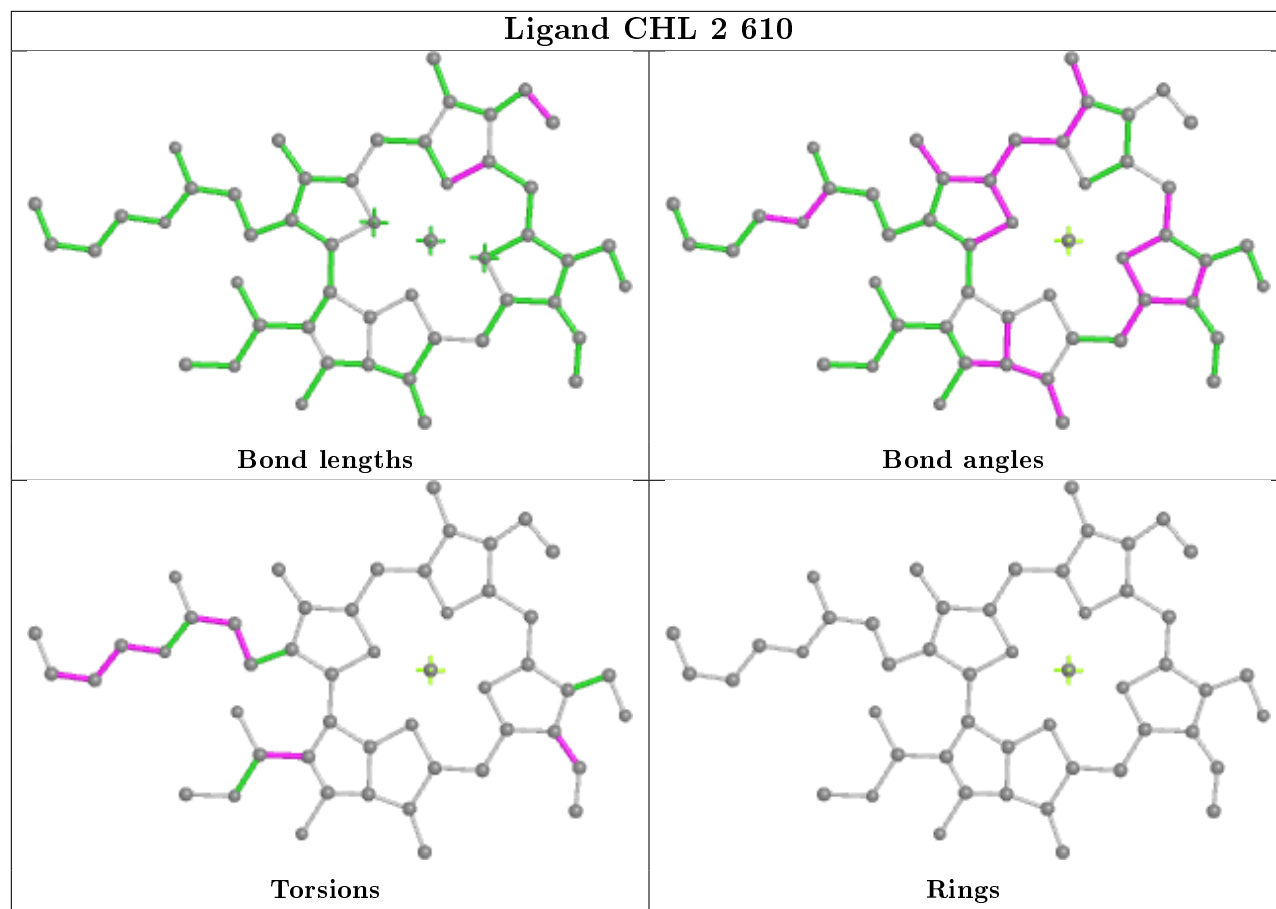


Torsions

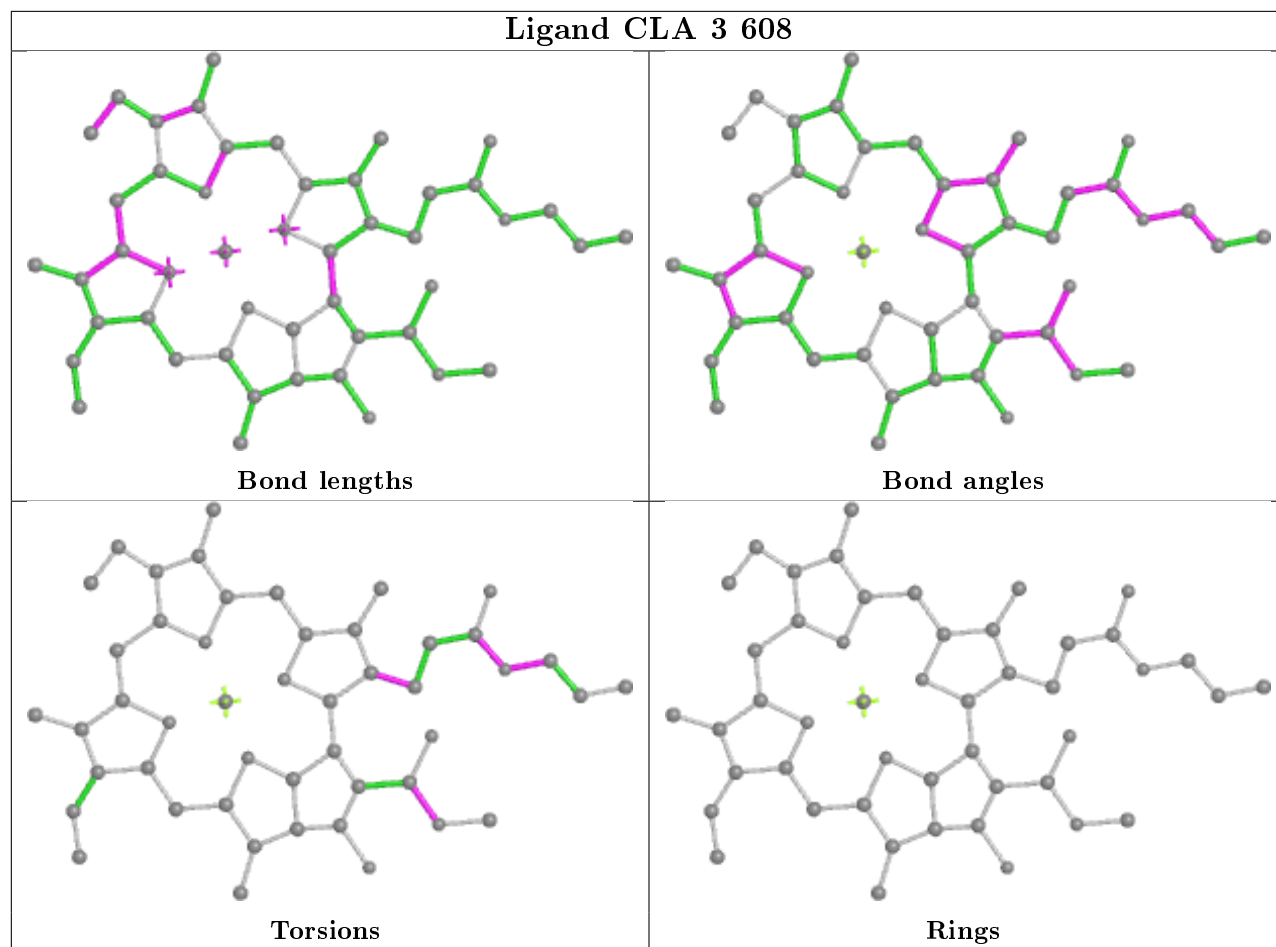


Rings

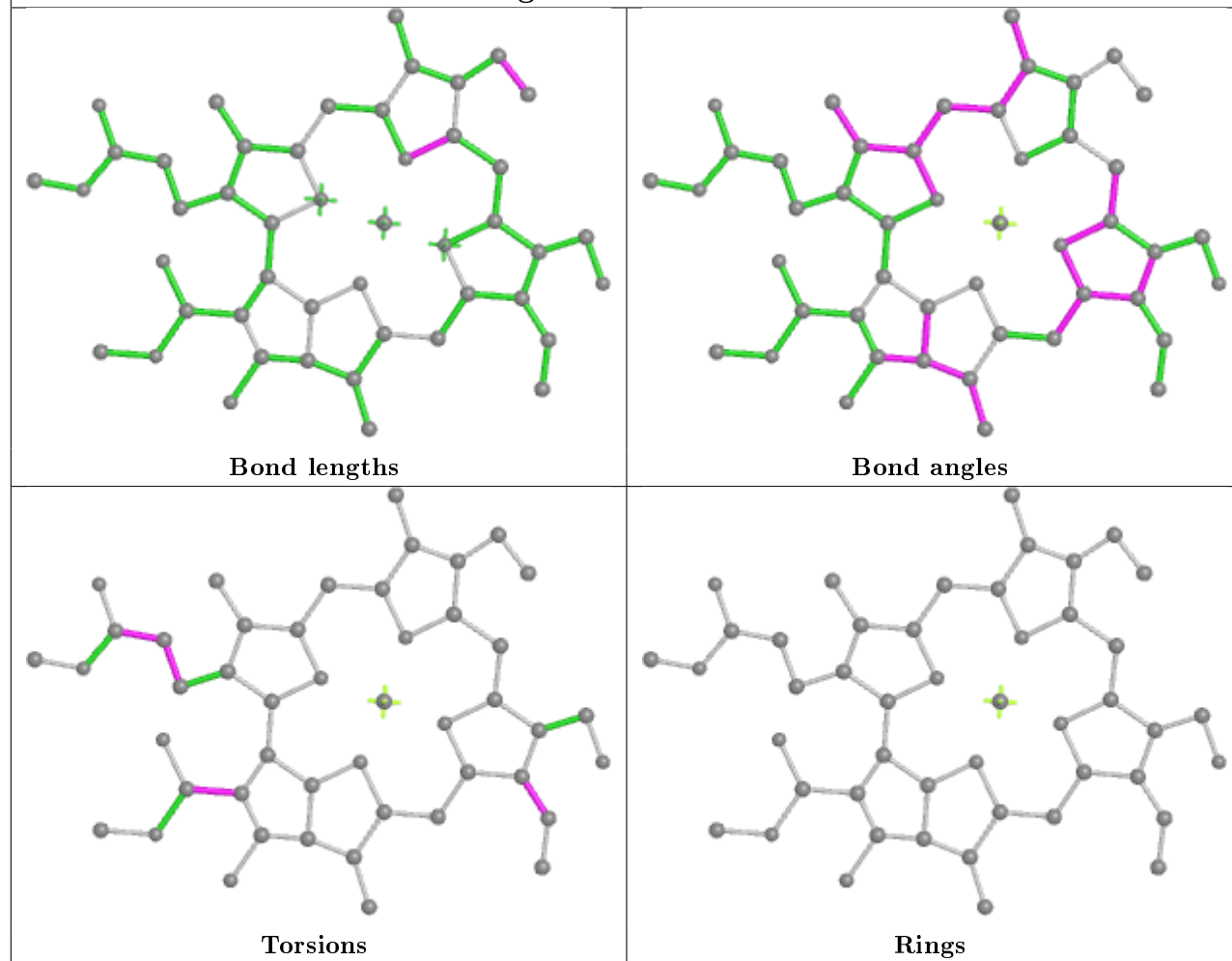
Ligand CHL 2 610

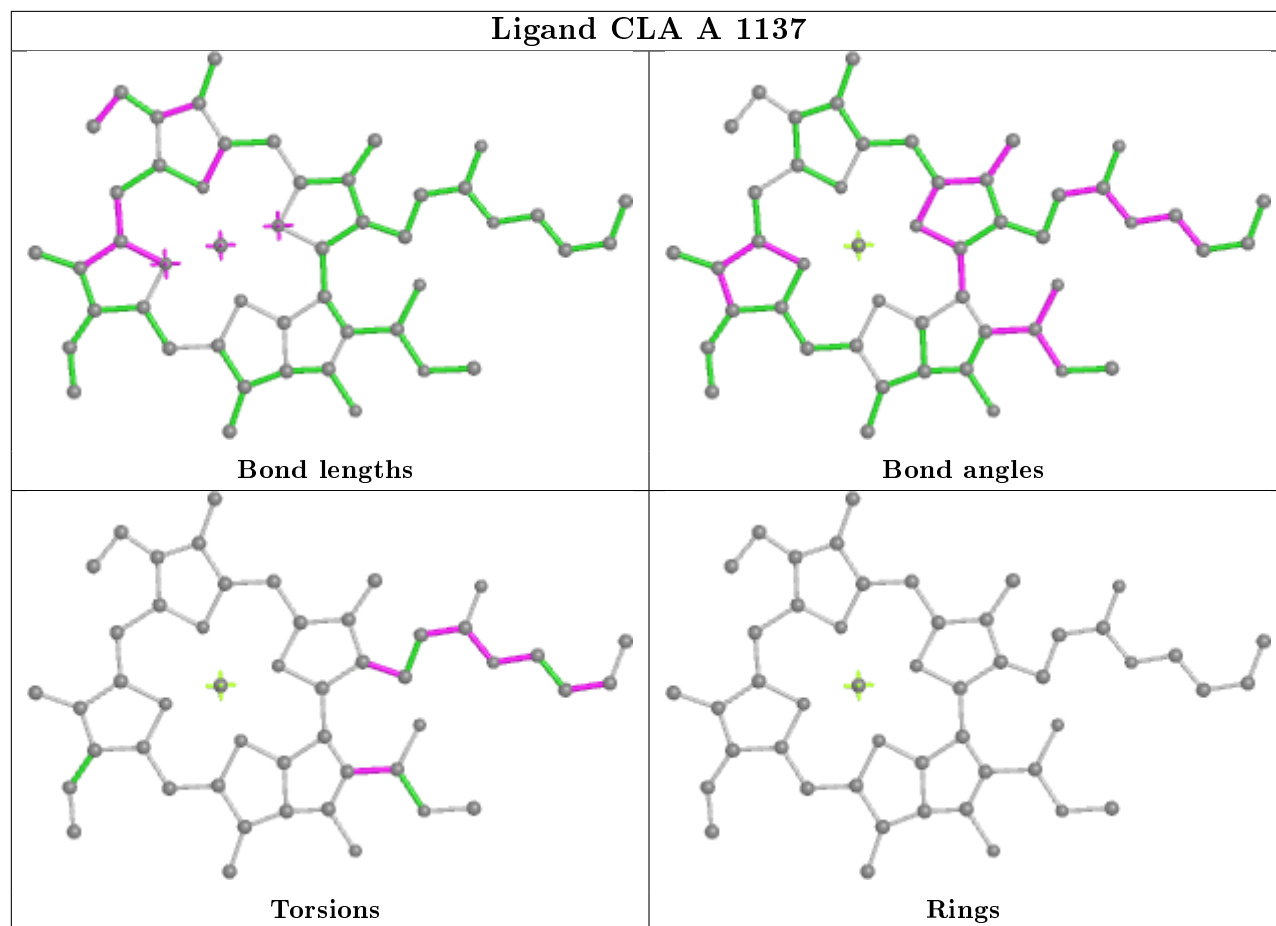


Ligand CLA 3 608

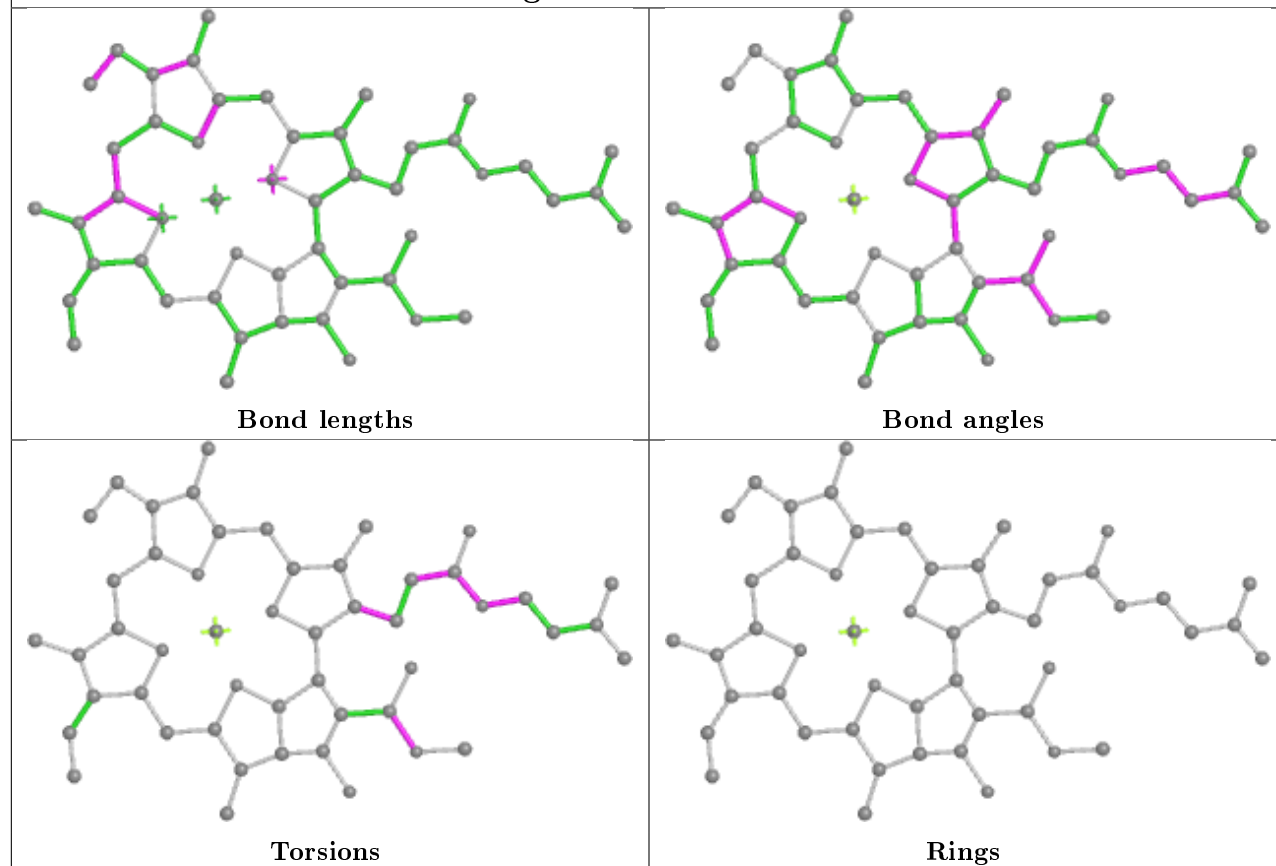


Ligand CHL 3 604

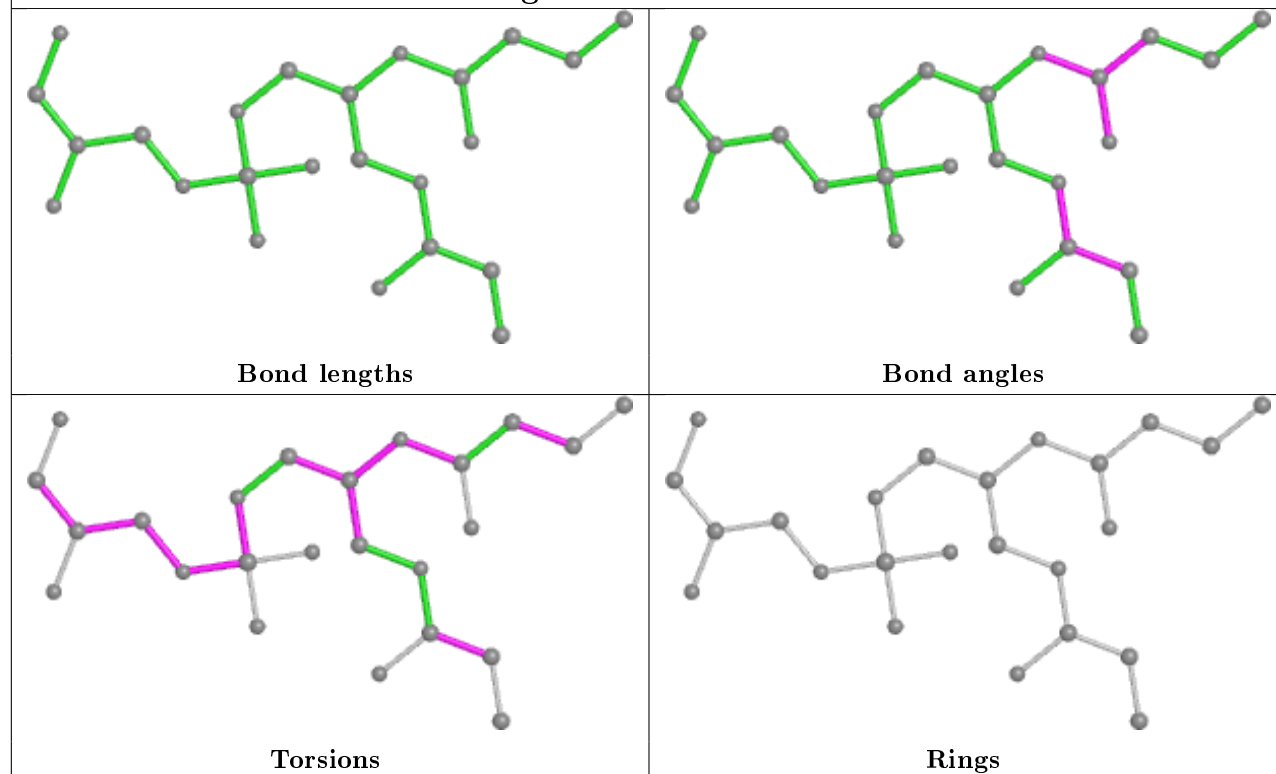


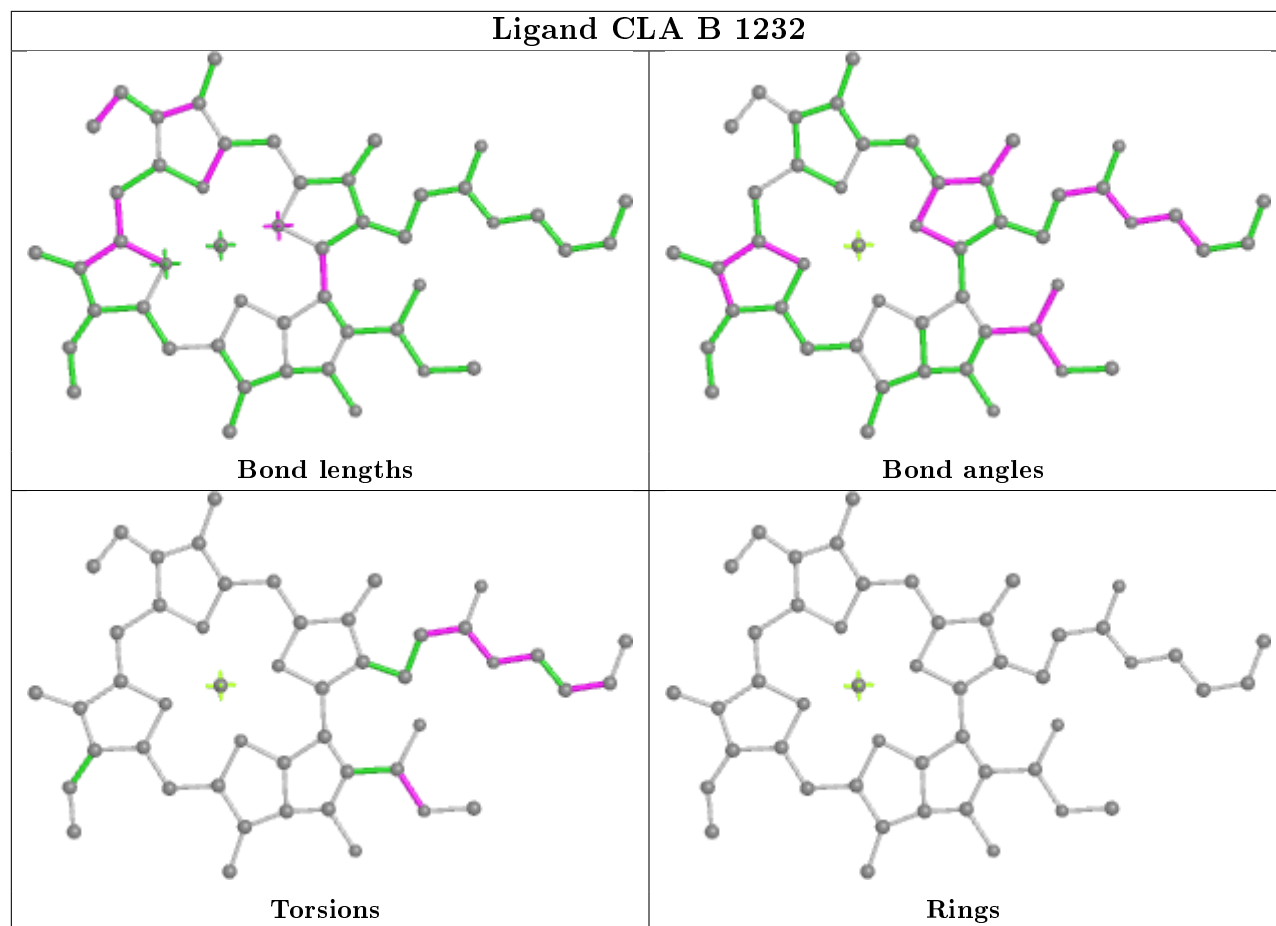


Ligand CLA B 1238

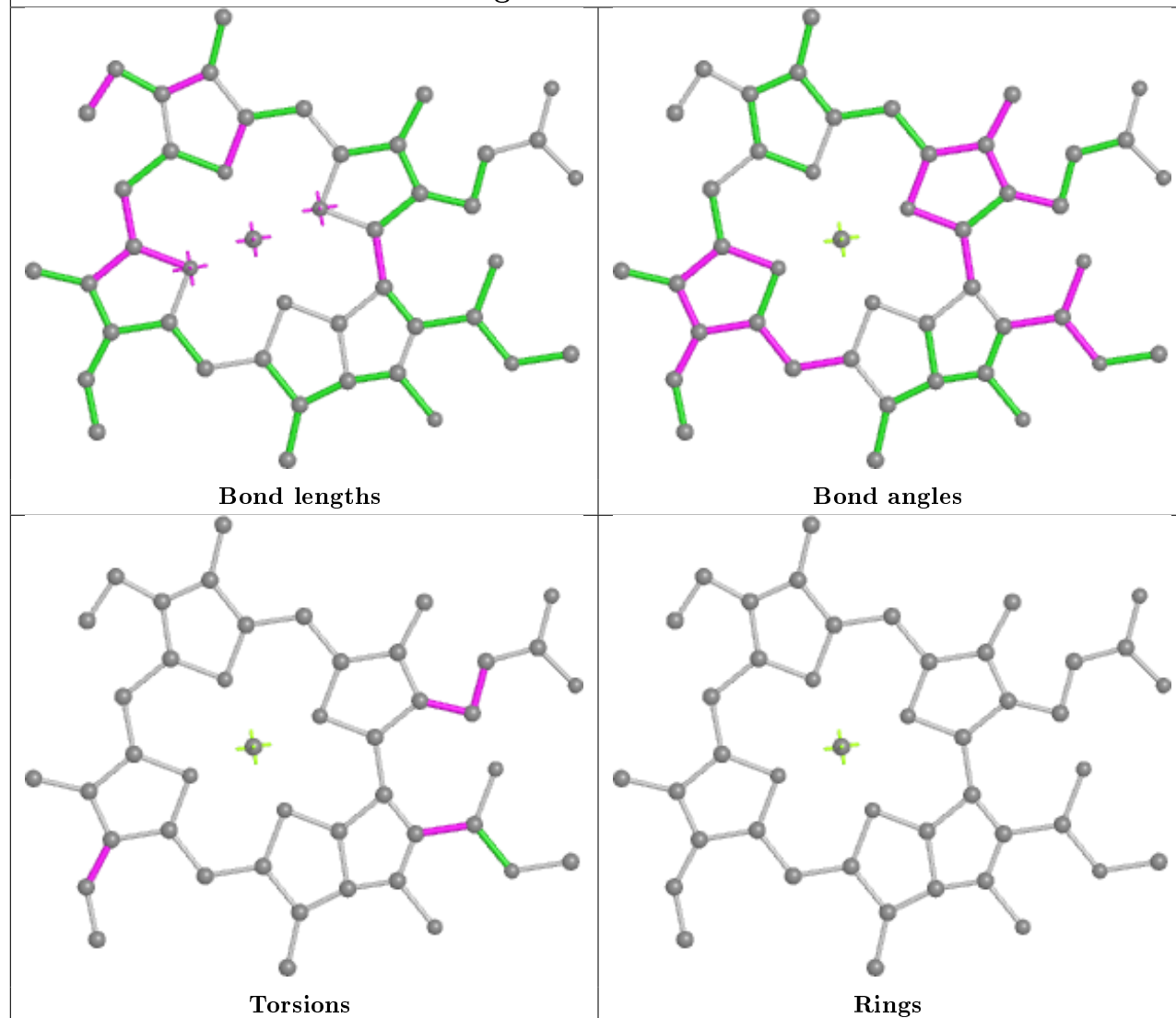


Ligand LHG A 5002

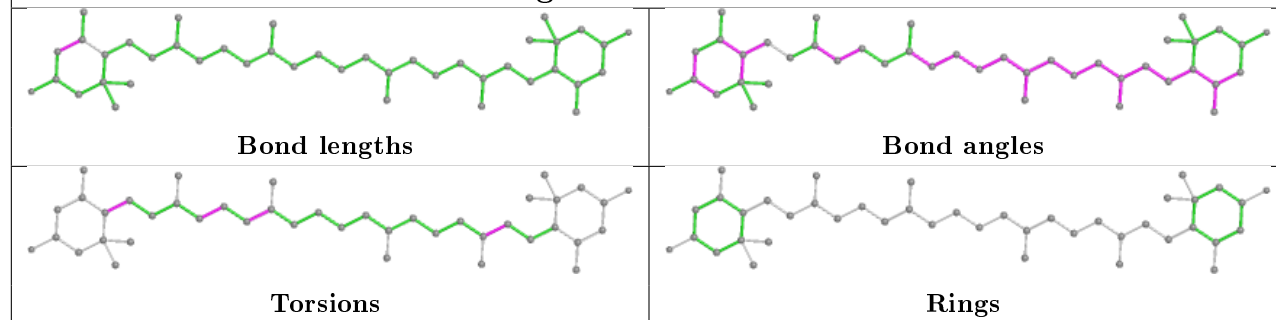


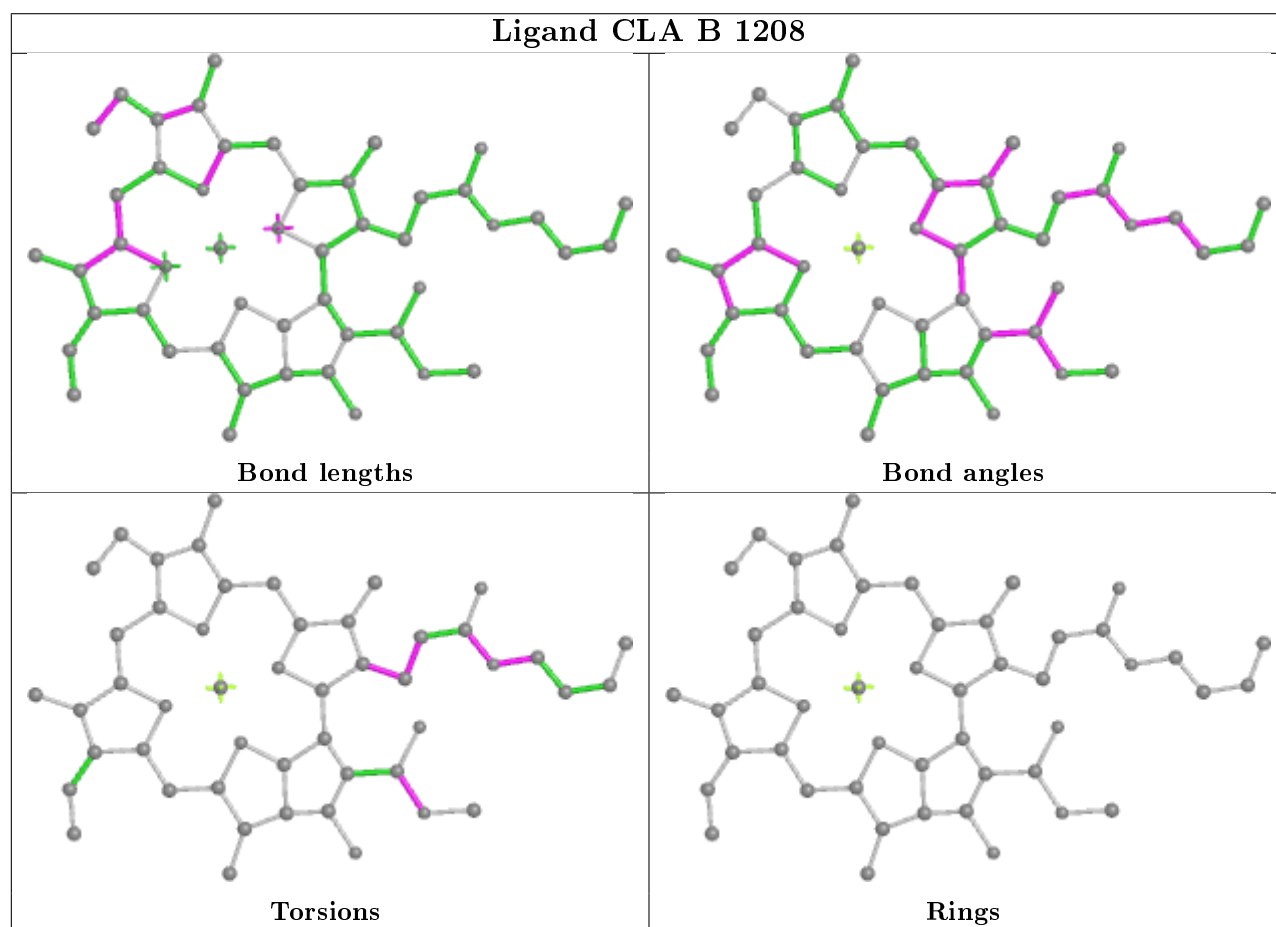
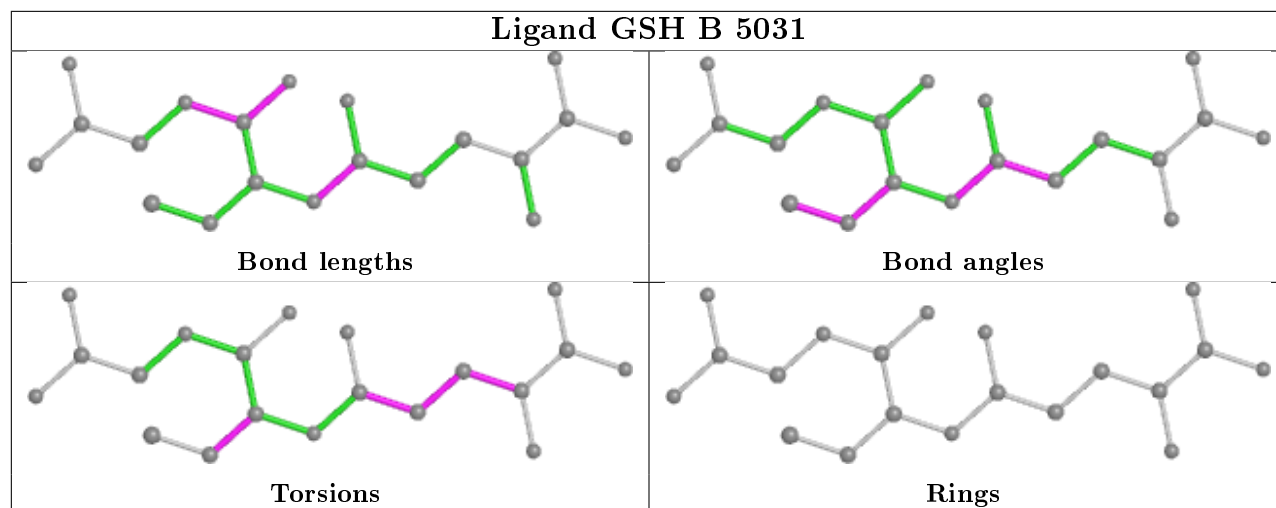


Ligand CLA 3 603

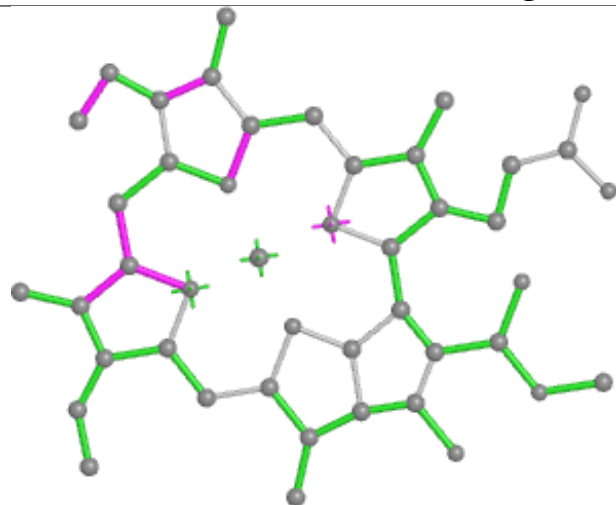


Ligand LUT 2 501

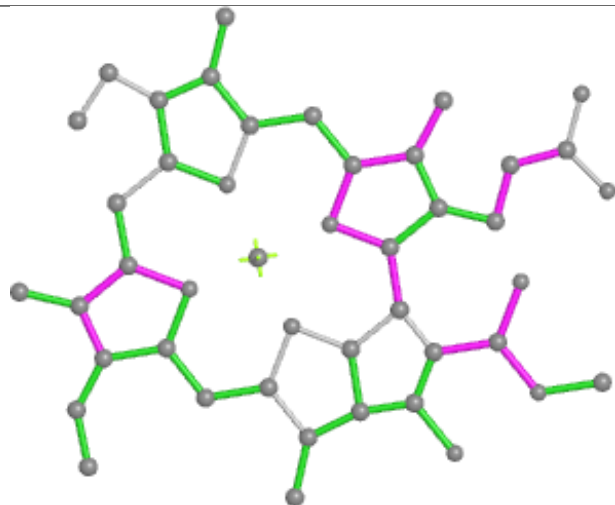




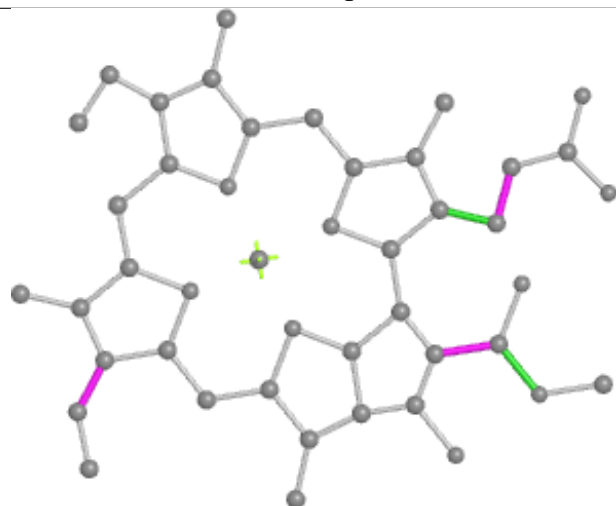
Ligand CLA 3 606



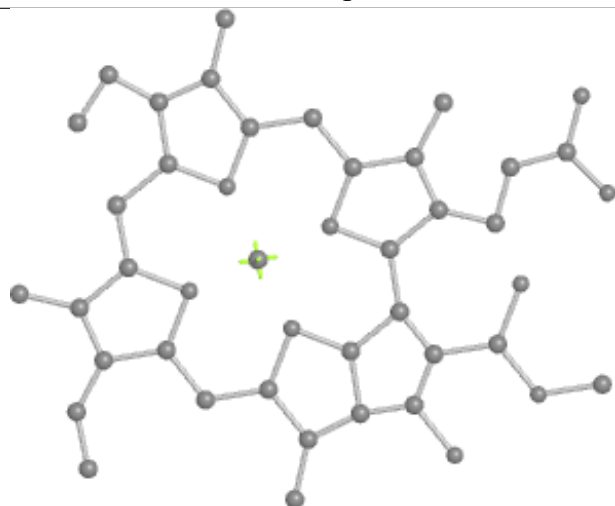
Bond lengths



Bond angles

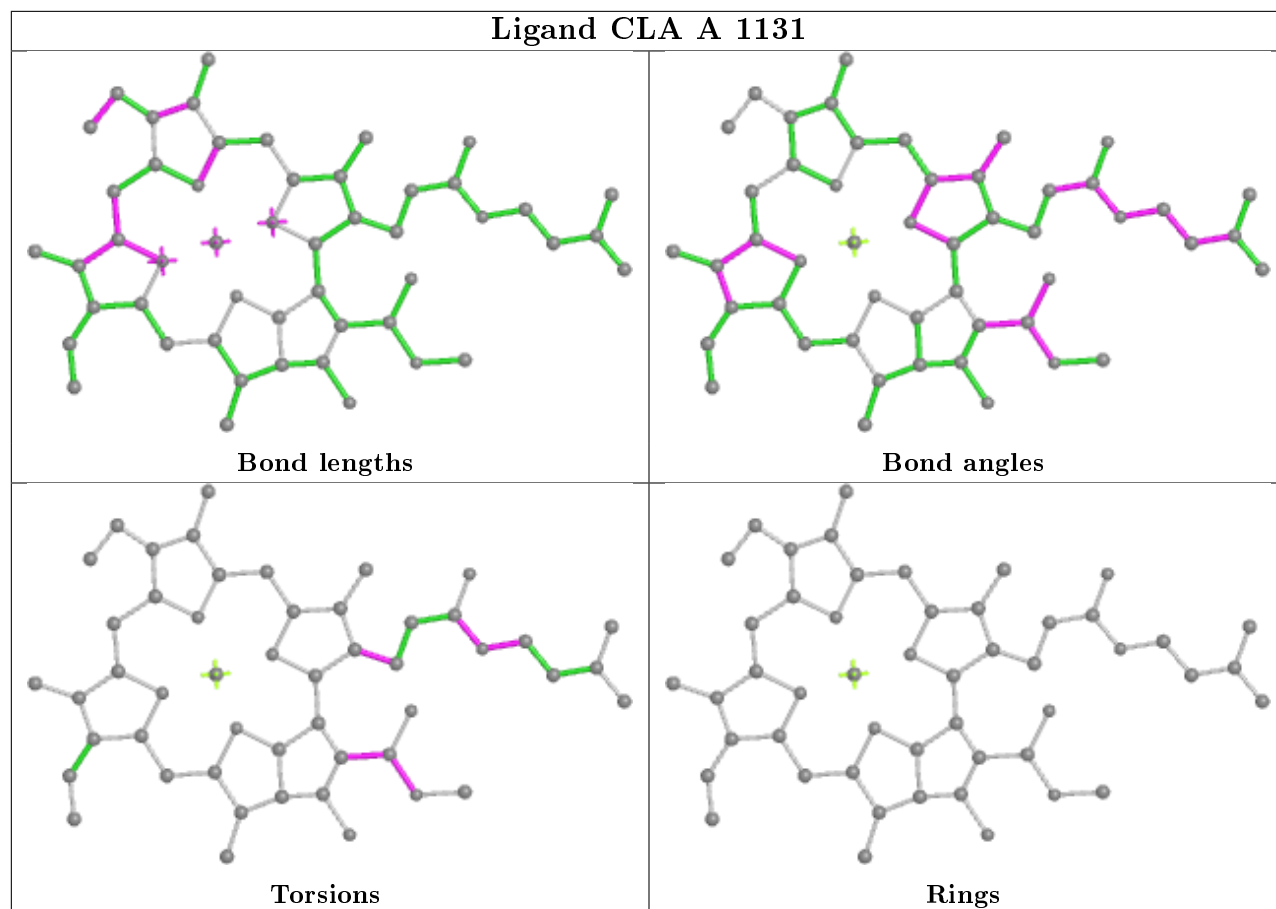


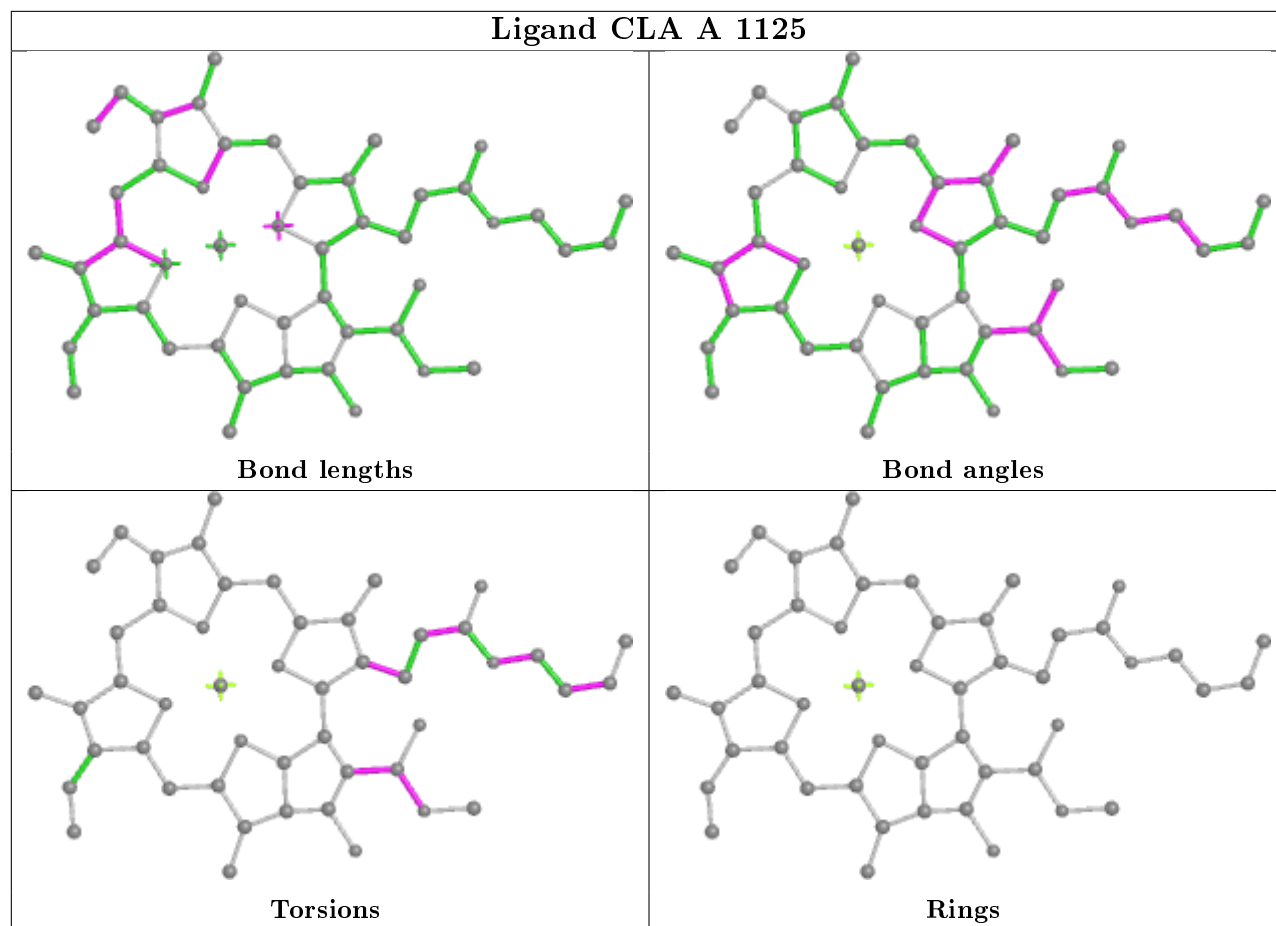
Torsions

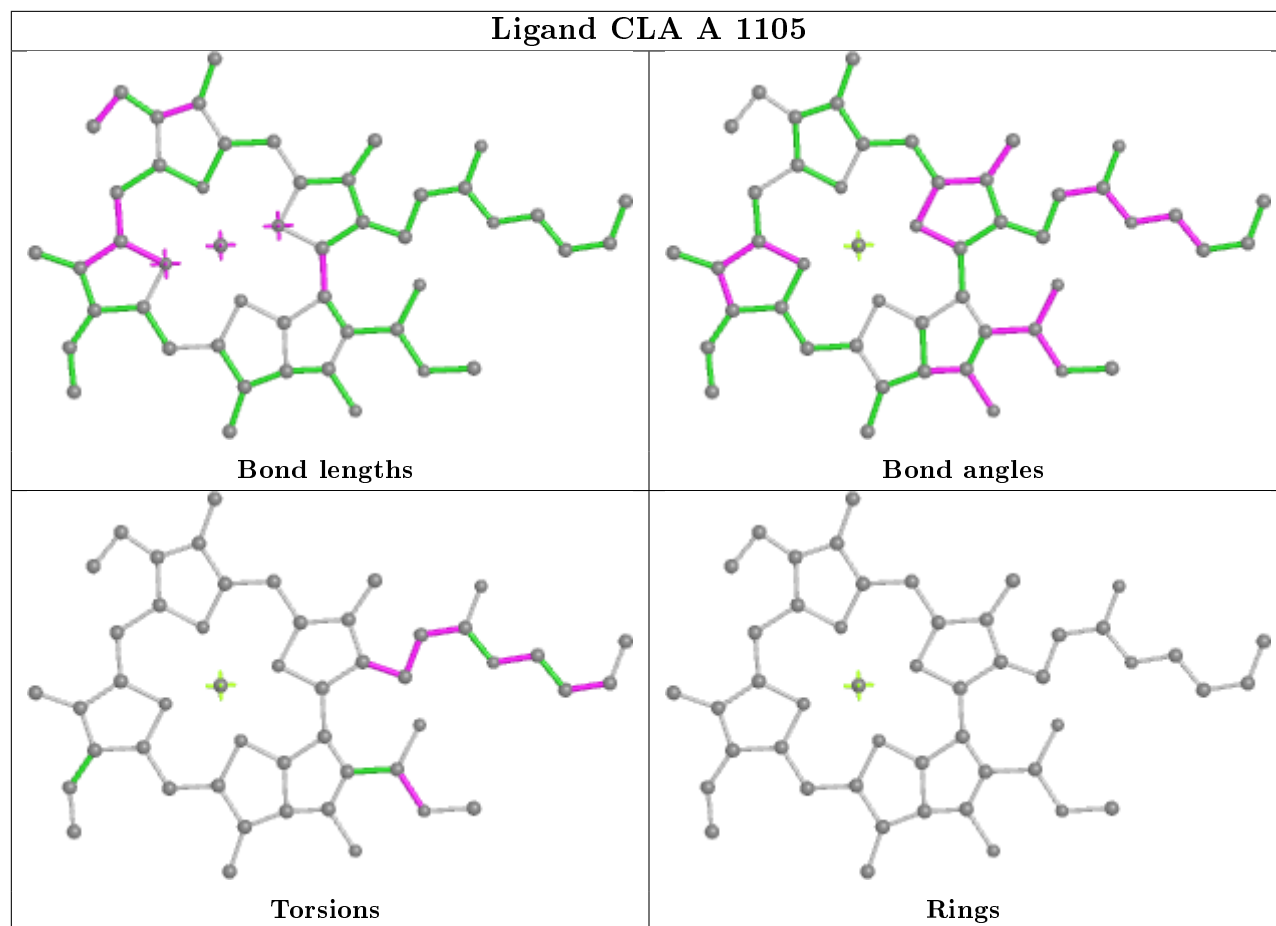


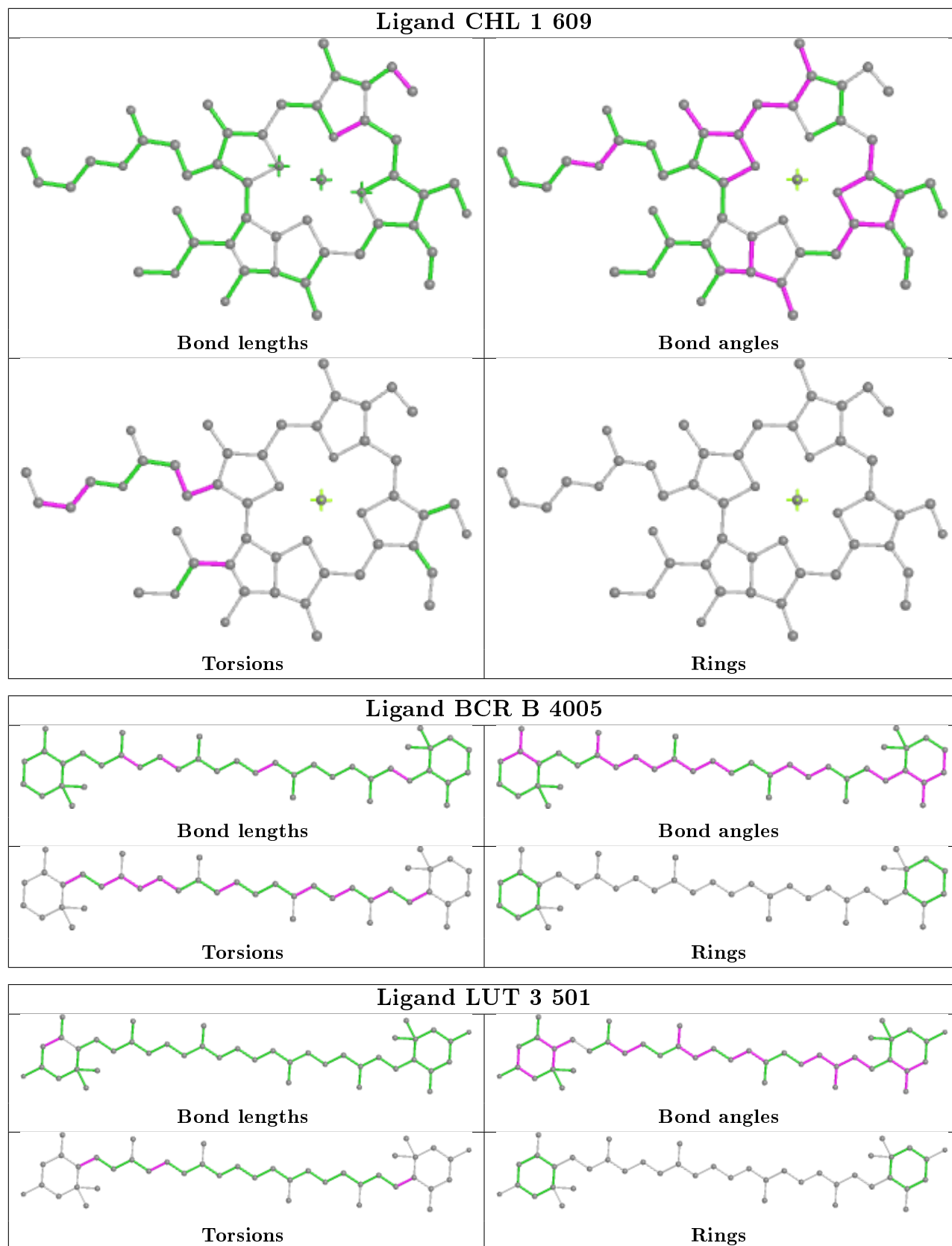
Rings

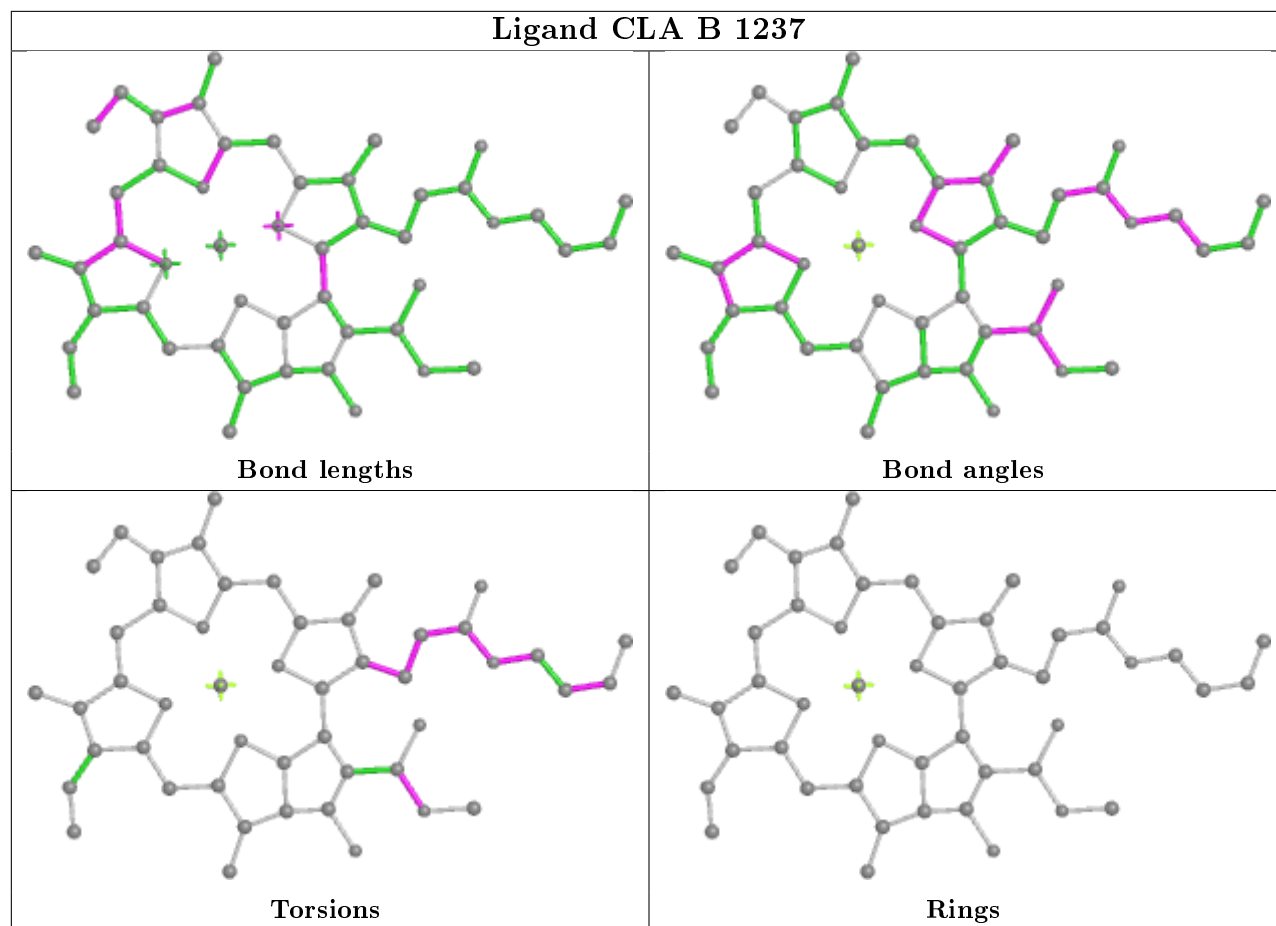
Ligand CLA A 1131



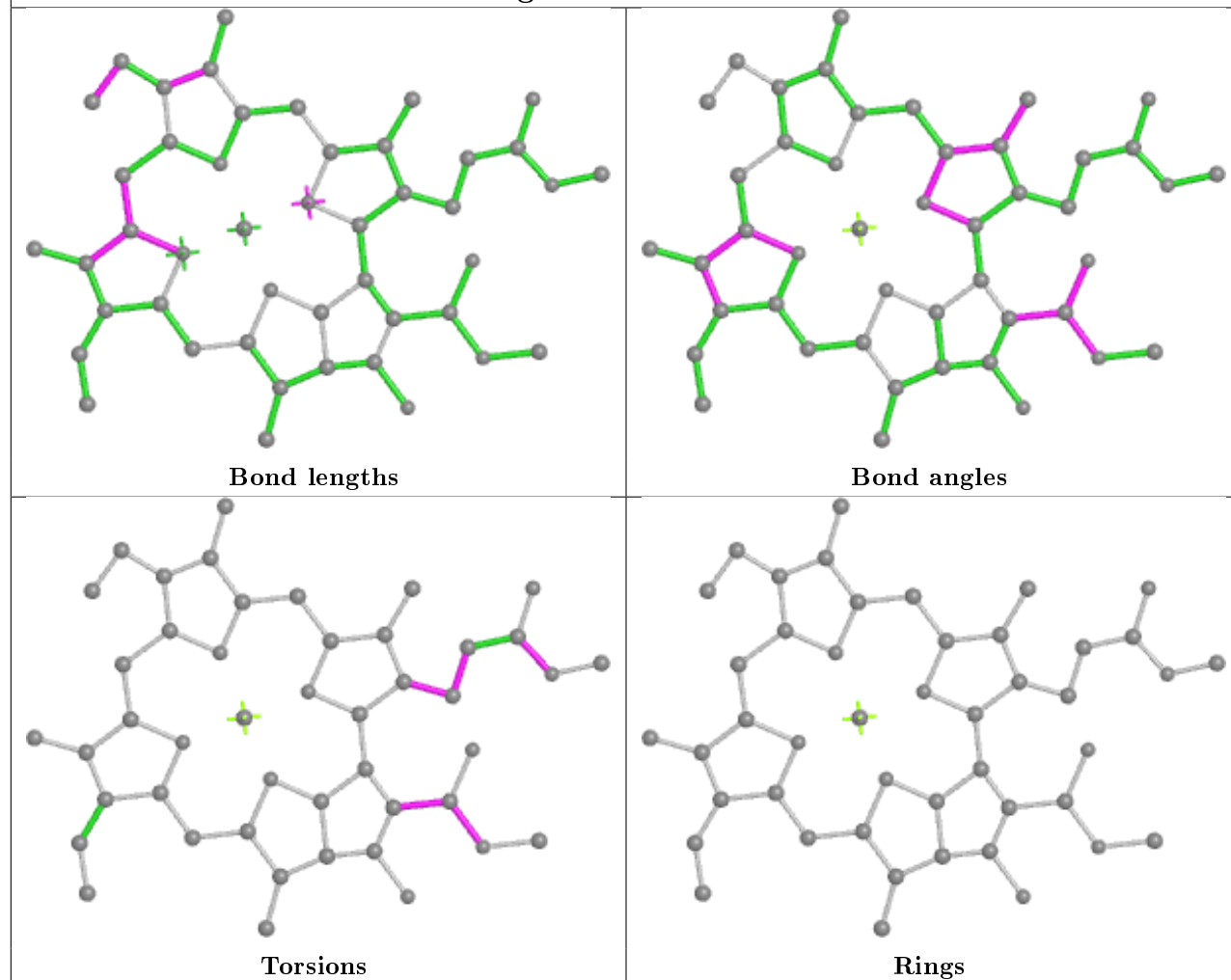




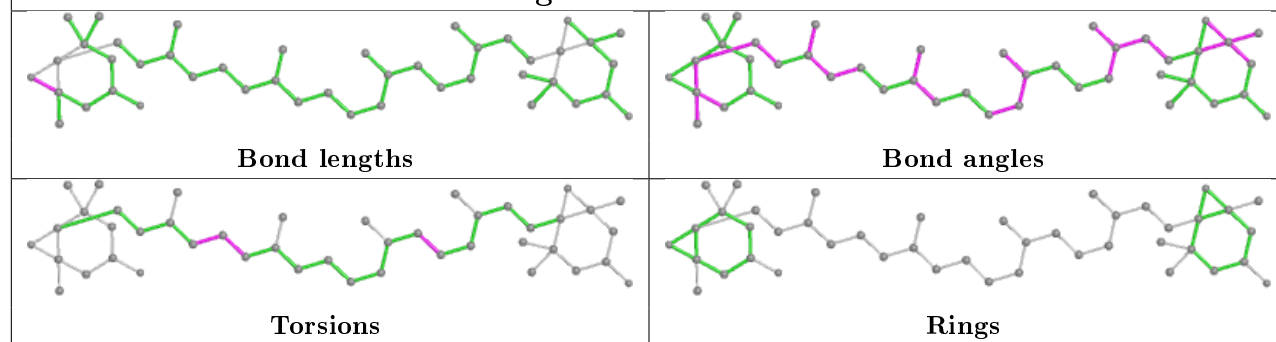




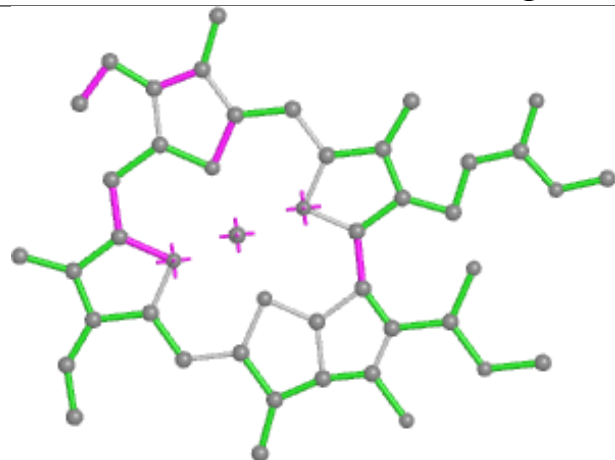
Ligand CLA 3 611



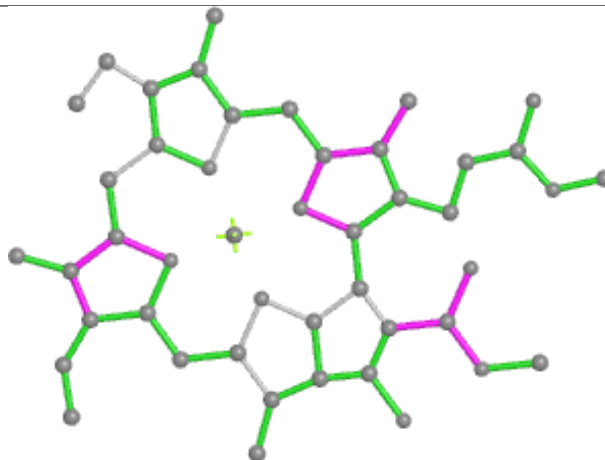
Ligand XAT 1 502



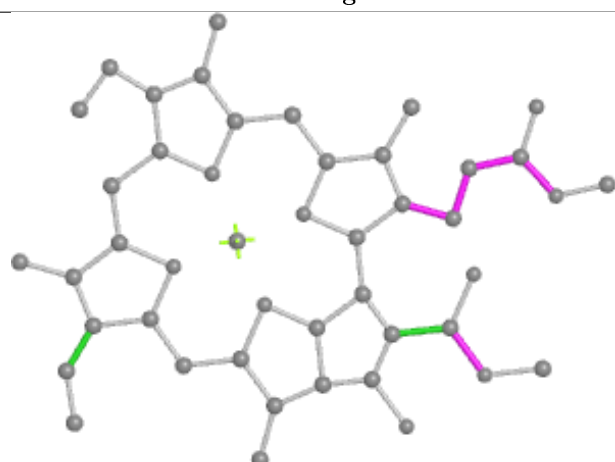
Ligand CLA 1 607



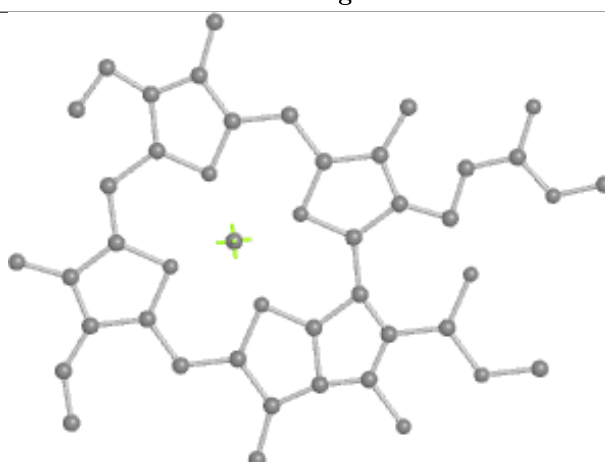
Bond lengths



Bond angles

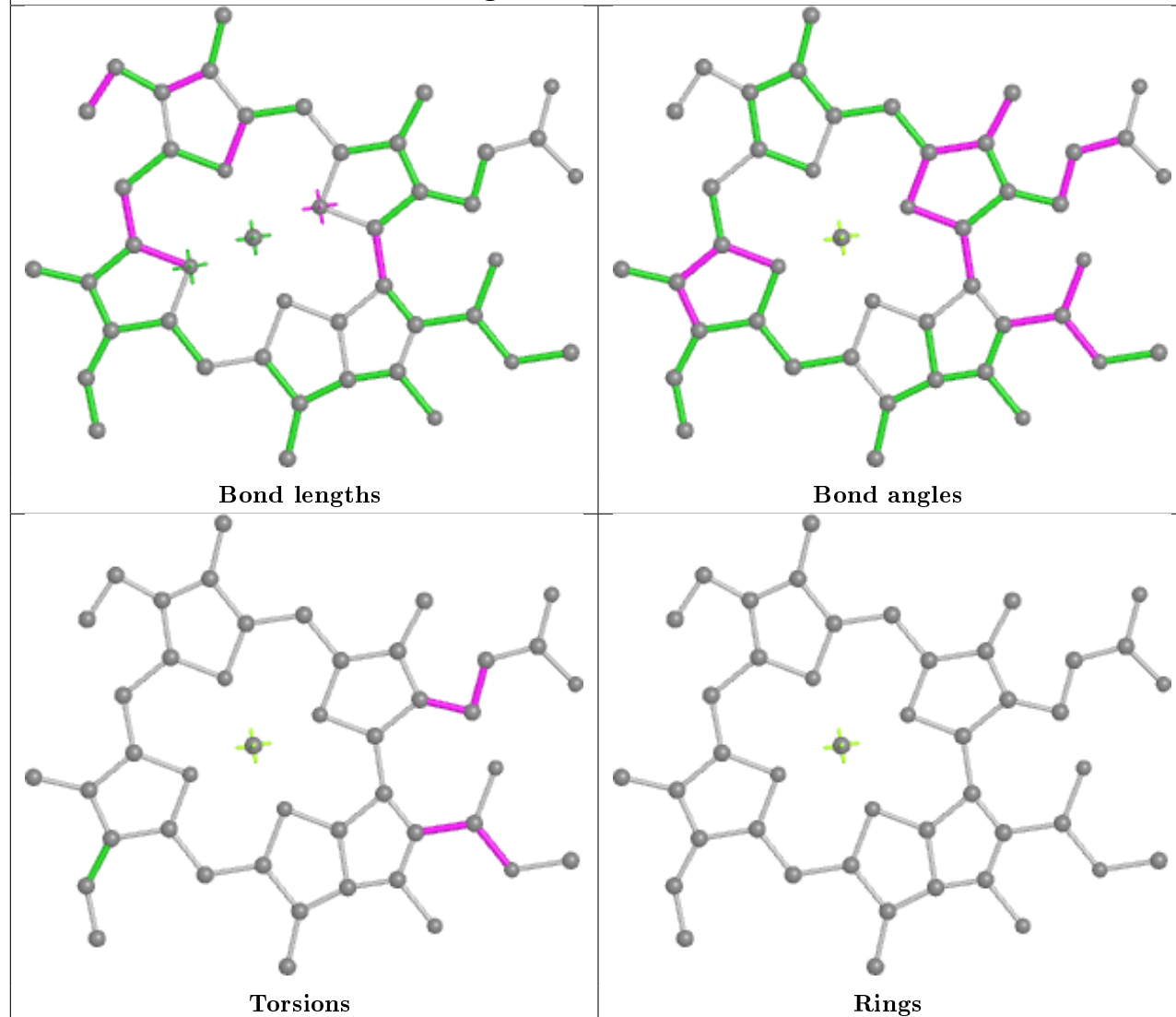


Torsions

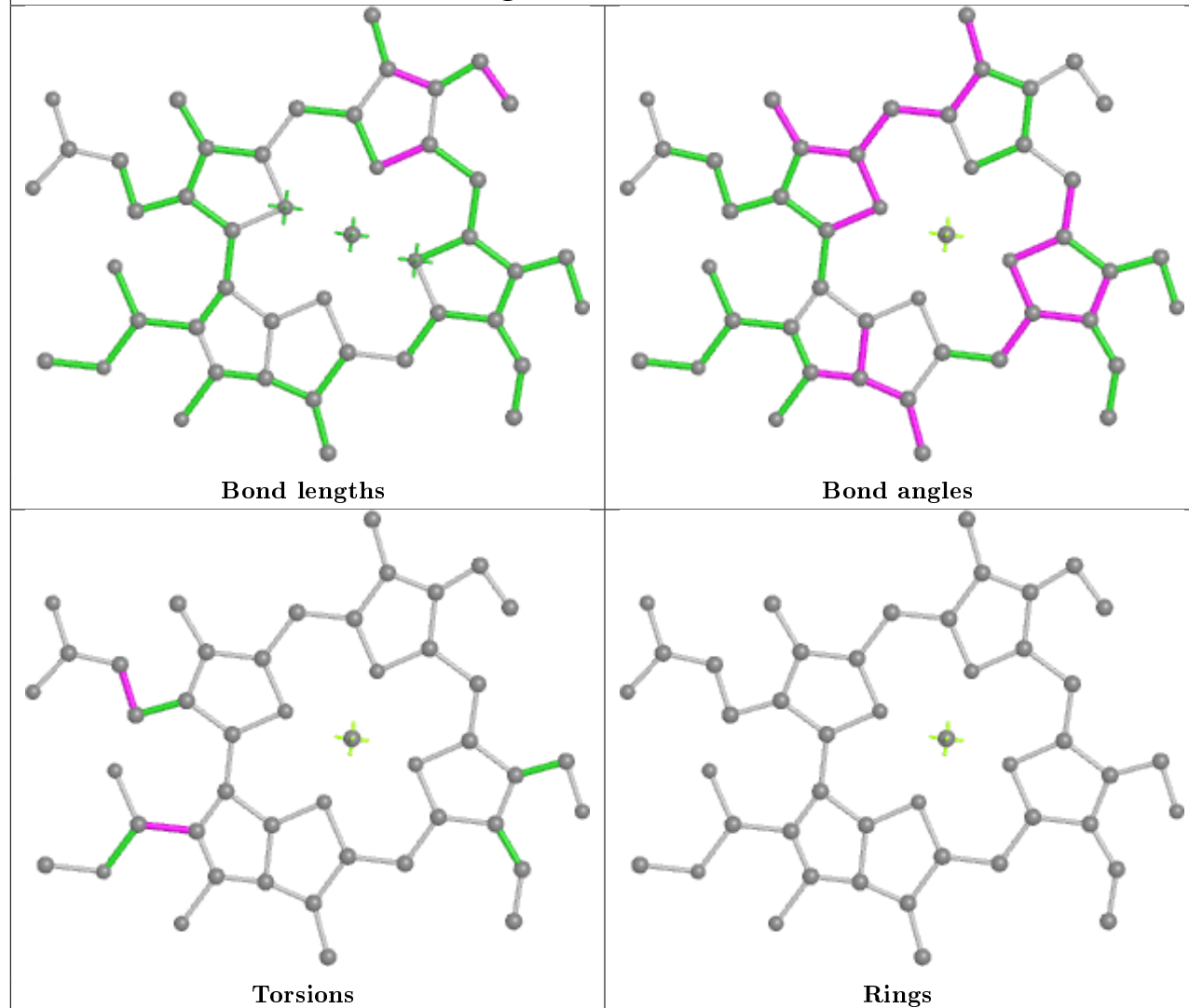


Rings

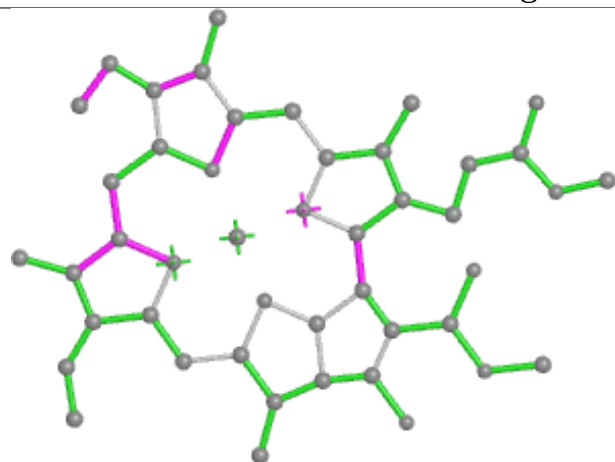
Ligand CLA B 1212



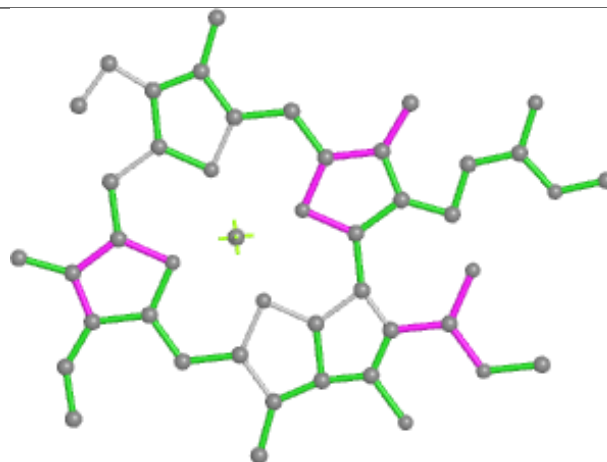
Ligand CHL 2 613



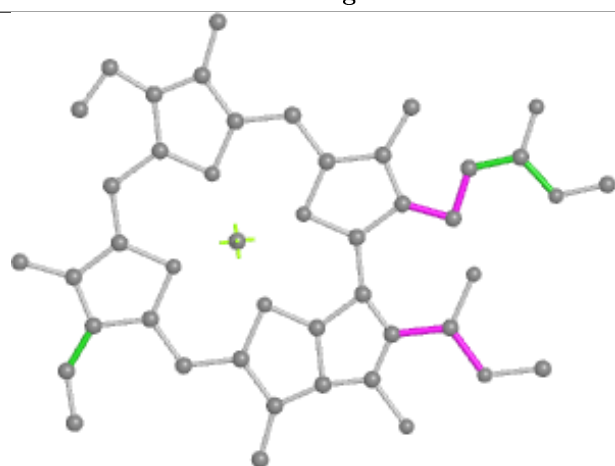
Ligand CLA 2 606



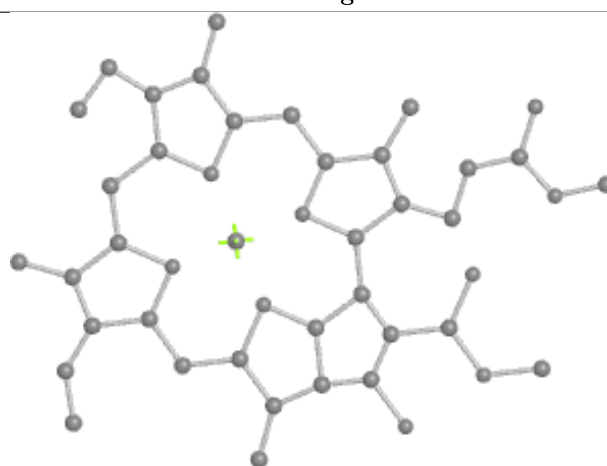
Bond lengths



Bond angles

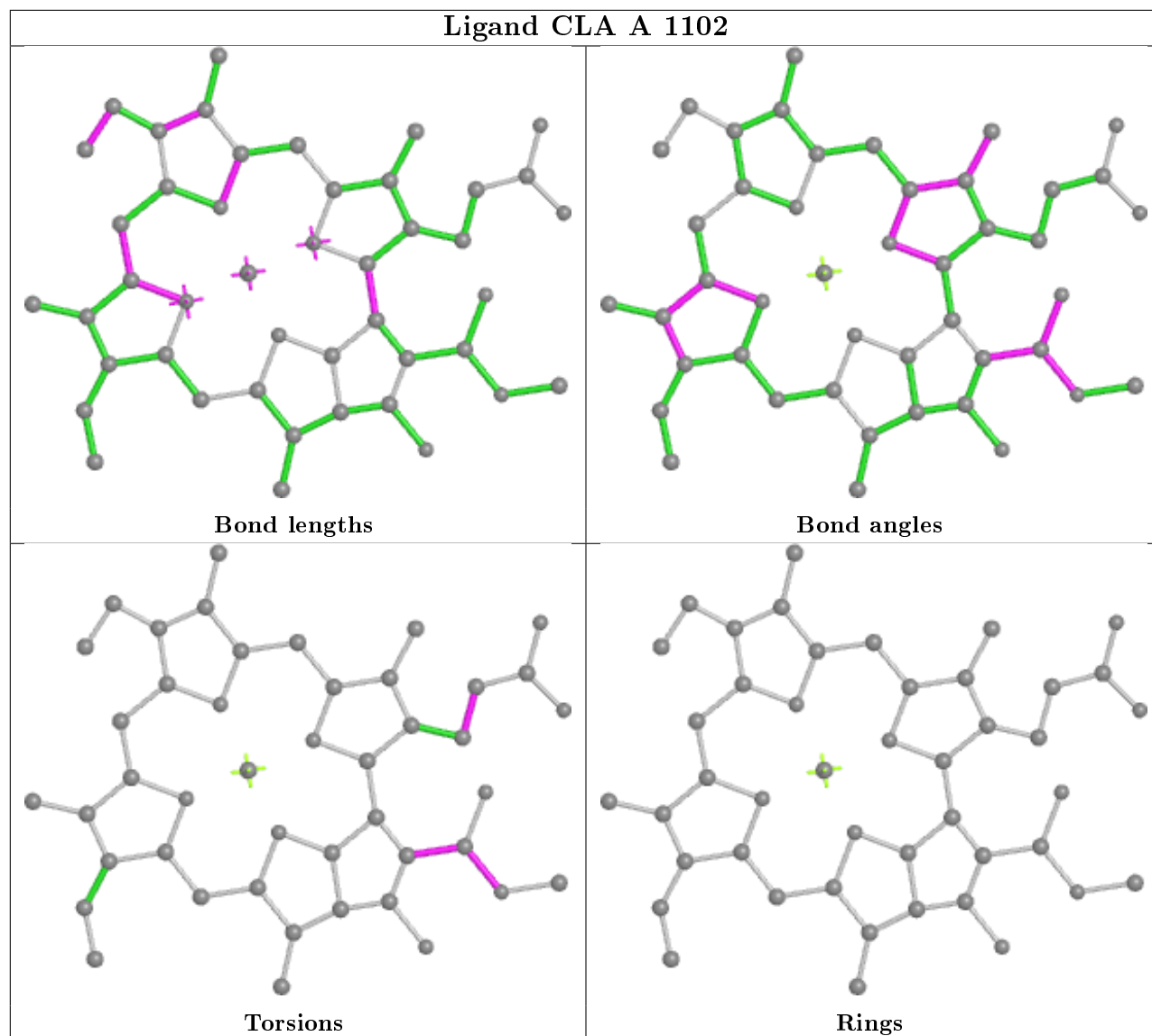


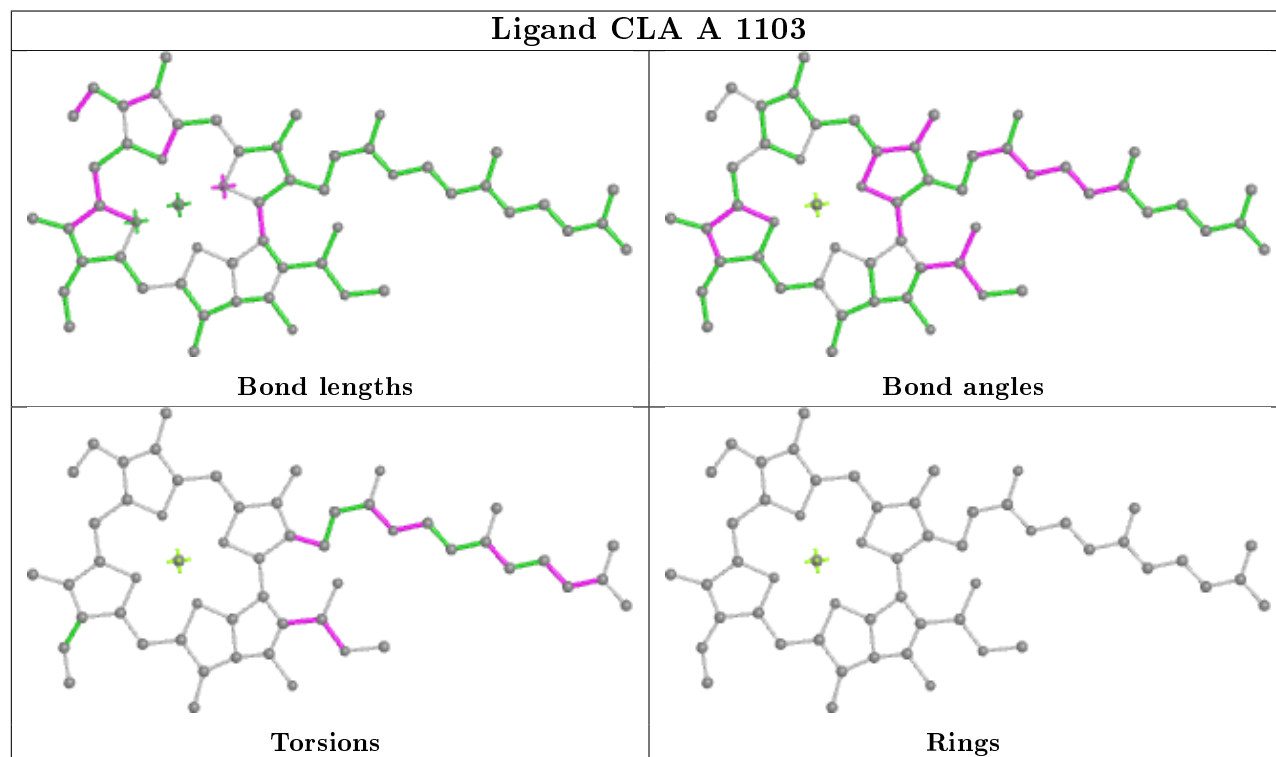
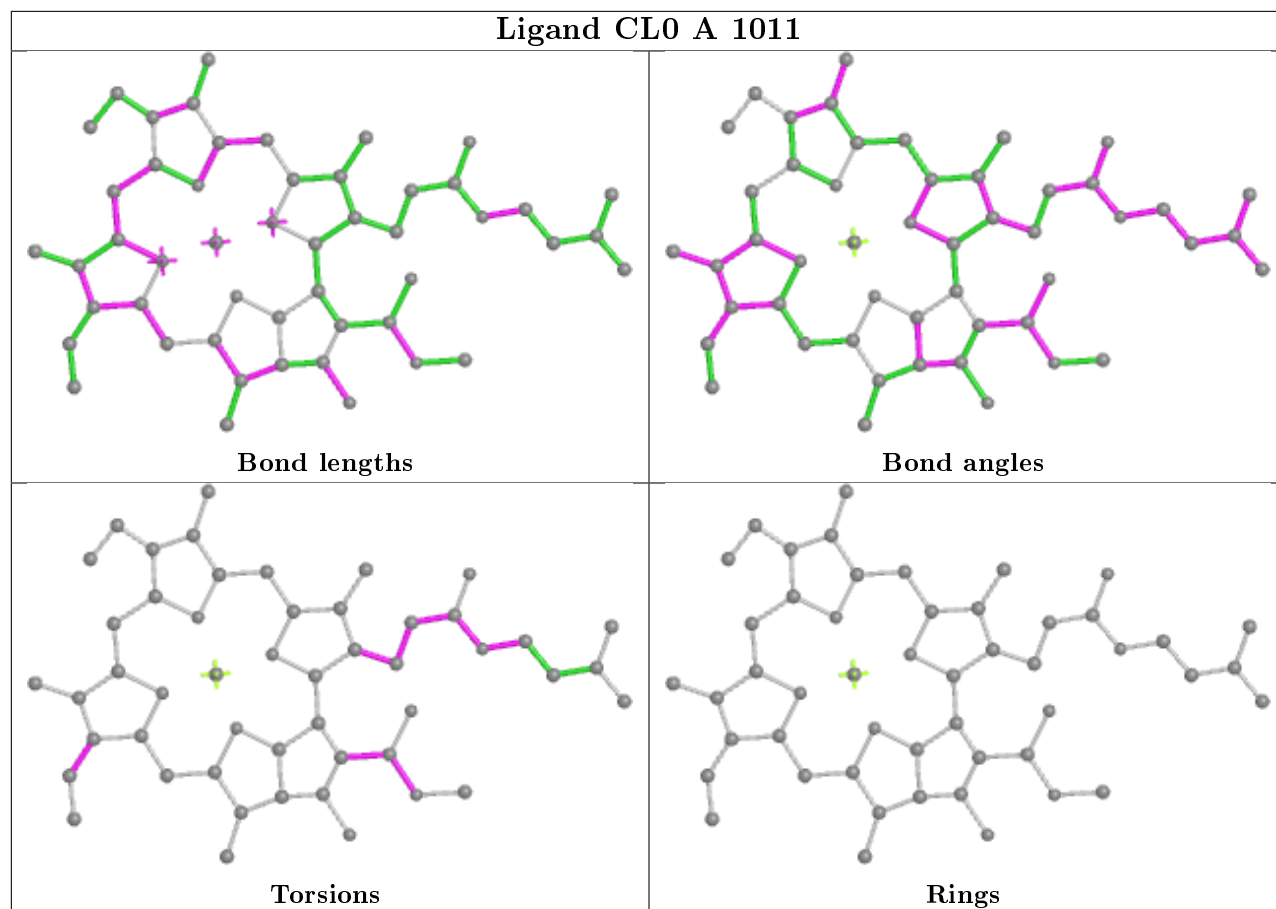
Torsions



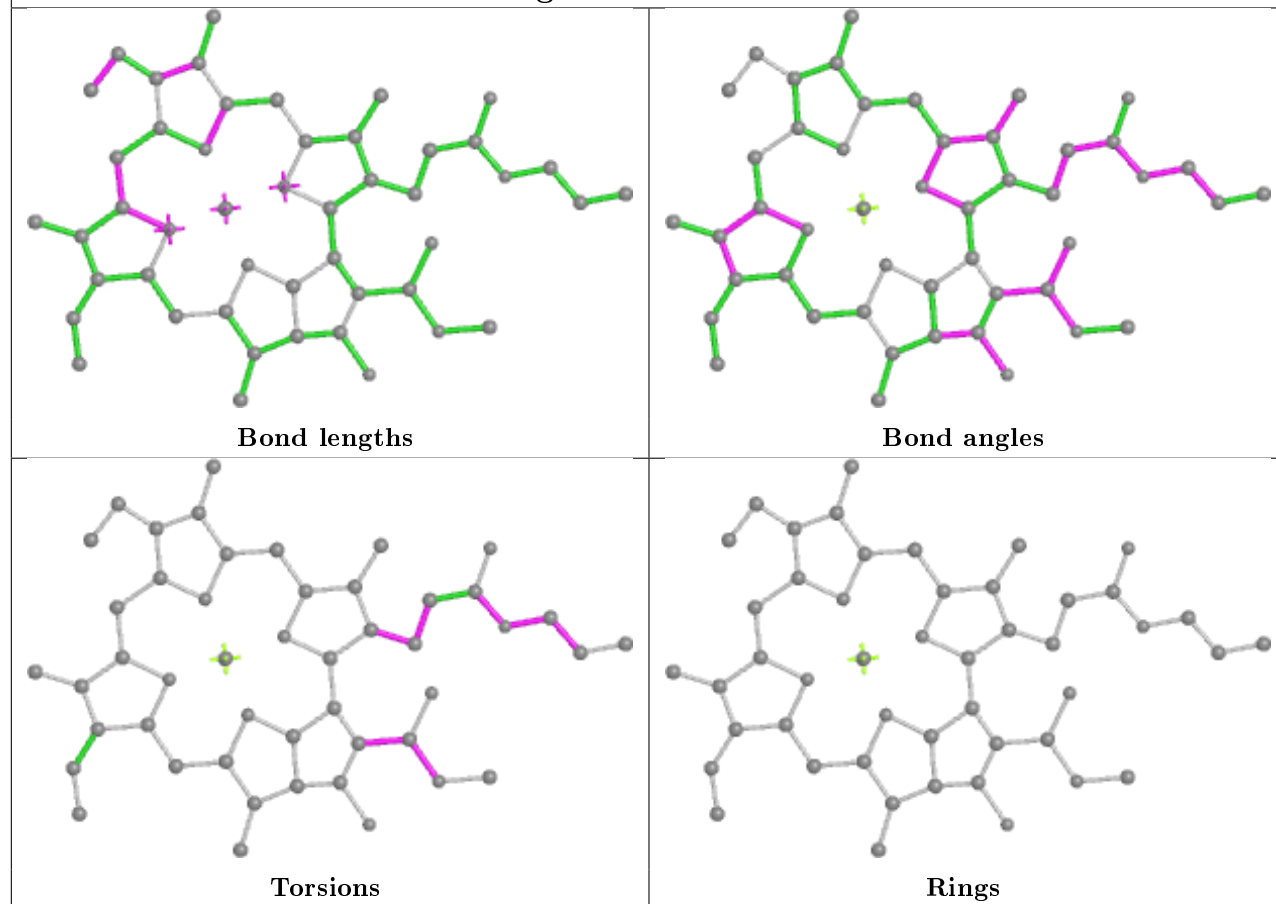
Rings

Ligand CLA A 1102

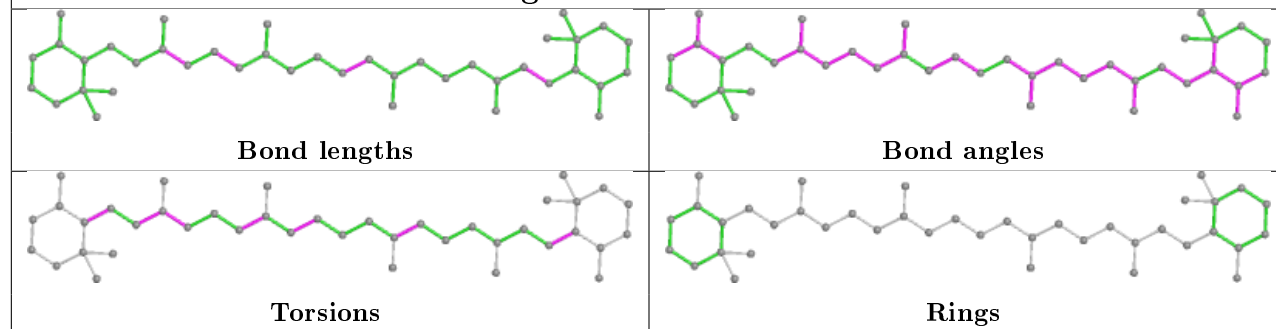


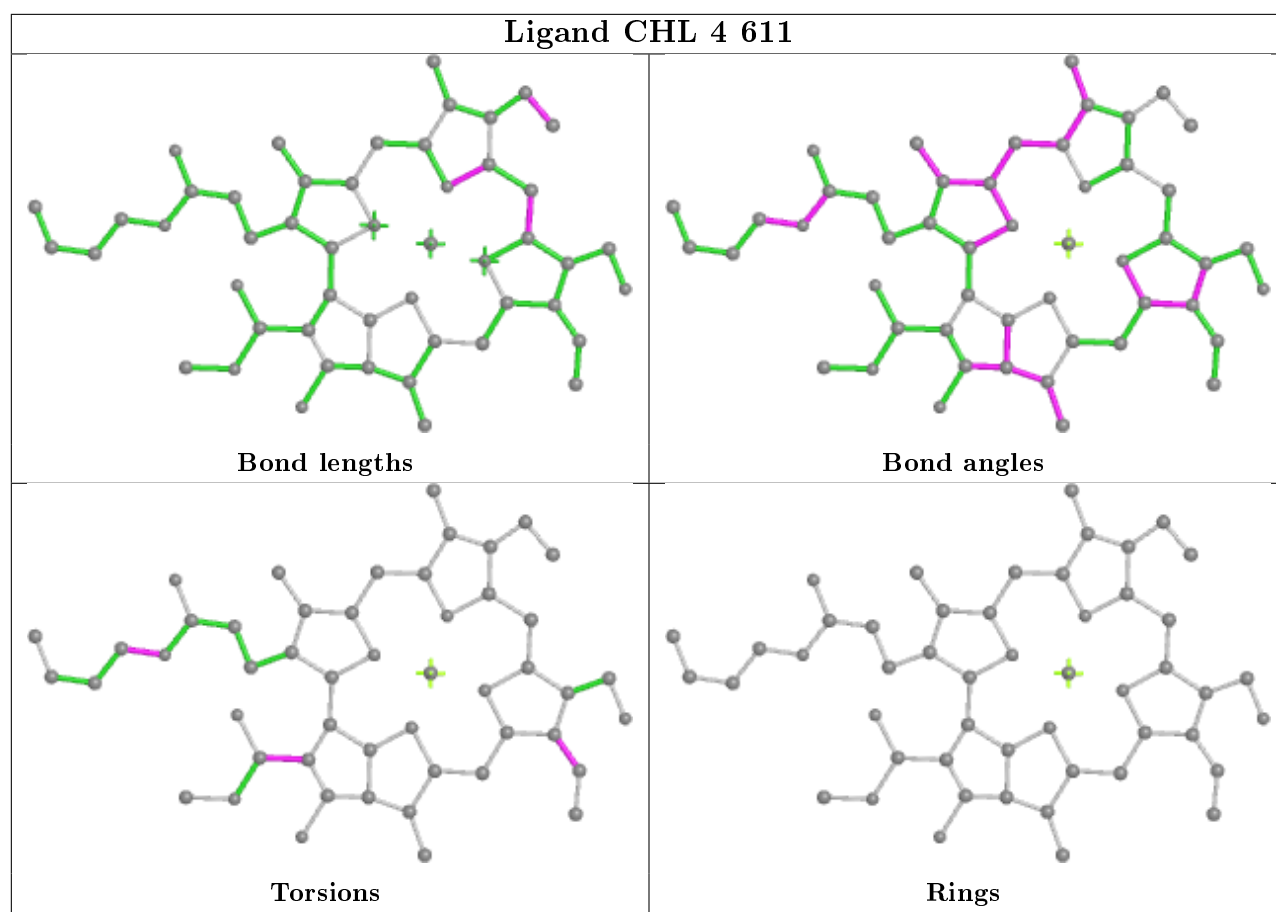


Ligand CLA 1 605



Ligand BCR A 4002





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	195/195 (100%)	0.73	36 (18%) 1 1	85, 106, 128, 134	0
2	2	211/211 (100%)	0.59	33 (15%) 2 2	91, 115, 138, 155	0
3	3	210/210 (100%)	1.12	47 (22%) 0 1	134, 167, 199, 210	0
4	4	211/211 (100%)	0.60	26 (12%) 4 5	84, 93, 107, 125	0
5	A	739/739 (100%)	0.71	100 (13%) 3 4	84, 127, 168, 187	0
6	B	734/734 (100%)	0.73	117 (15%) 1 2	83, 114, 149, 180	0
7	C	80/80 (100%)	1.17	20 (25%) 0 0	104, 128, 142, 146	0
8	D	142/142 (100%)	1.46	42 (29%) 0 0	108, 153, 174, 189	0
9	E	64/64 (100%)	0.44	6 (9%) 8 10	93, 103, 115, 120	0
10	F	163/163 (100%)	0.03	7 (4%) 35 35	80, 87, 99, 105	0
11	J	41/41 (100%)	0.62	8 (19%) 1 1	82, 87, 103, 105	0
All	All	2790/2790 (100%)	0.73	442 (15%) 2 2	80, 117, 171, 210	0

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	506	THR	21.0
3	3	96	ASN	20.0
6	B	735	GLY	18.7
8	D	112	ILE	15.6
8	D	120	ALA	15.4
8	D	84	PHE	13.5
8	D	121	ALA	13.4
5	A	280	GLY	12.8
8	D	85	GLY	12.7
6	B	2	ALA	12.6
5	A	505	ALA	12.2
5	A	420	THR	11.8

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Mol	Chain	Res	Type	RSRZ
5	A	510	TRP	10.2
3	3	91	ASP	10.2
5	A	511	GLY	10.2
5	A	281	GLY	10.0
5	A	507	SER	9.9
6	B	733	ARG	9.8
5	A	292	SER	9.6
4	4	182	PHE	9.0
6	B	4	LYS	8.8
3	3	75	ASP	8.8
3	3	98	GLN	8.5
6	B	731	ALA	8.5
8	D	209	PRO	8.3
6	B	188	SER	8.3
8	D	114	GLU	8.0
6	B	41	GLU	8.0
3	3	73	TYR	7.9
8	D	113	PHE	7.6
8	D	119	GLY	7.6
4	4	208	ASP	7.5
3	3	92	PRO	7.2
8	D	99	GLU	7.2
8	D	86	GLY	7.1
3	3	84	PHE	6.9
5	A	282	LEU	6.9
5	A	421	ASN	6.9
6	B	734	PHE	6.8
4	4	211	THR	6.7
2	2	189	ASP	6.7
6	B	11	GLN	6.7
6	B	601	THR	6.7
5	A	289	LEU	6.7
5	A	377	TYR	6.7
5	A	418	ASP	6.5
4	4	209	ASN	6.5
2	2	207	GLY	6.4
3	3	141	ALA	6.4
6	B	84	HIS	6.4
8	D	98	GLU	6.4
6	B	45	GLN	6.3
3	3	137	GLY	6.2
3	3	140	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
6	B	35	HIS	6.2
4	4	269	TYR	6.1
6	B	3	THR	6.0
3	3	88	GLY	6.0
5	A	384	TYR	6.0
6	B	334	GLN	6.0
11	J	1	MET	5.9
10	F	236	ASN	5.9
5	A	266	THR	5.9
2	2	210	LYS	5.8
6	B	15	GLN	5.7
5	A	279	LYS	5.7
3	3	103	PHE	5.6
5	A	294	THR	5.6
2	2	212	GLU	5.6
8	D	94	LYS	5.6
7	C	76	SER	5.6
2	2	215	PHE	5.6
5	A	422	ASN	5.6
1	1	111	ASP	5.5
6	B	732	GLY	5.4
6	B	692	VAL	5.4
1	1	91	ALA	5.4
2	2	214	SER	5.4
8	D	122	ILE	5.4
4	4	178	VAL	5.4
3	3	112	SER	5.3
2	2	208	MET	5.3
6	B	304	ALA	5.2
6	B	691	LEU	5.2
5	A	496	GLN	5.2
3	3	95	SER	5.2
2	2	217	GLU	5.2
6	B	653	PHE	5.2
5	A	504	ALA	5.1
3	3	89	LEU	5.1
4	4	186	PHE	5.1
5	A	268	ASN	5.1
4	4	194	LEU	5.0
3	3	111	TYR	5.0
2	2	260	HIS	5.0
8	D	132	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
6	B	694	TRP	5.0
6	B	368	THR	4.9
5	A	157	LEU	4.9
5	A	260	GLY	4.9
6	B	333	PHE	4.9
2	2	161	LEU	4.9
5	A	508	LEU	4.9
8	D	196	VAL	4.8
6	B	394	PHE	4.7
1	1	210	LEU	4.7
5	A	293	ASP	4.7
3	3	97	GLY	4.7
10	F	232	GLU	4.7
6	B	727	ILE	4.7
5	A	270	ALA	4.7
1	1	188	CYS	4.6
7	C	27	GLU	4.6
6	B	42	ASN	4.6
11	J	2	LYS	4.6
2	2	271	PRO	4.6
3	3	132	ILE	4.5
7	C	50	GLY	4.5
3	3	74	LEU	4.5
1	1	214	PHE	4.5
5	A	275	PHE	4.5
3	3	76	GLY	4.4
3	3	282	THR	4.4
6	B	693	TYR	4.4
4	4	128	TYR	4.4
11	J	4	PHE	4.4
5	A	291	LEU	4.3
9	E	111	TYR	4.3
4	4	189	ILE	4.2
2	2	244	HIS	4.2
3	3	104	VAL	4.2
3	3	80	GLY	4.2
6	B	9	PHE	4.2
7	C	6	LYS	4.2
2	2	211	ASN	4.2
8	D	130	LEU	4.2
3	3	90	LEU	4.2
5	A	497	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	1	126	THR	4.1
6	B	690	ASN	4.1
5	A	375	PRO	4.1
5	A	749	ALA	4.1
1	1	55	ASN	4.1
8	D	138	CYS	4.1
1	1	81	TRP	4.1
8	D	185	VAL	4.1
4	4	242	ASP	4.0
4	4	250	ASP	4.0
9	E	127	VAL	4.0
5	A	503	LEU	4.0
5	A	750	VAL	4.0
6	B	665	LEU	4.0
6	B	14	ALA	4.0
6	B	331	LEU	4.0
5	A	615	GLN	4.0
7	C	32	ASP	4.0
2	2	216	LYS	4.0
8	D	95	ALA	4.0
6	B	687	PRO	3.9
5	A	689	GLY	3.9
4	4	172	TRP	3.9
5	A	290	TRP	3.9
6	B	44	TYR	3.9
6	B	360	ALA	3.9
6	B	12	GLY	3.8
2	2	256	ALA	3.8
5	A	687	PHE	3.8
1	1	164	SER	3.8
1	1	112	LYS	3.8
5	A	267	LEU	3.8
5	A	509	THR	3.8
6	B	18	SER	3.8
4	4	123	ASP	3.7
7	C	75	ARG	3.7
3	3	114	VAL	3.7
3	3	93	THR	3.7
6	B	87	PRO	3.7
5	A	493	THR	3.7
2	2	213	ALA	3.7
3	3	133	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	1	163	PHE	3.6
2	2	272	HIS	3.6
6	B	359	TYR	3.6
6	B	582	PHE	3.6
8	D	101	TYR	3.6
1	1	165	LYS	3.5
3	3	156	ALA	3.5
4	4	129	PRO	3.5
6	B	666	ILE	3.5
6	B	566	GLY	3.5
2	2	255	VAL	3.5
2	2	206	MET	3.5
5	A	528	LEU	3.5
11	J	3	ASP	3.5
2	2	162	PHE	3.5
5	A	359	LEU	3.5
6	B	714	PHE	3.5
5	A	26	PHE	3.4
6	B	139	SER	3.4
11	J	12	PRO	3.4
5	A	17	VAL	3.4
7	C	26	LEU	3.4
1	1	123	ASP	3.4
5	A	512	GLY	3.4
6	B	110	ALA	3.3
8	D	111	GLN	3.3
9	E	87	VAL	3.3
6	B	603	TRP	3.3
7	C	43	PRO	3.3
5	A	276	LEU	3.3
6	B	710	GLY	3.2
6	B	491	GLN	3.2
6	B	284	LEU	3.2
1	1	39	PRO	3.2
6	B	143	LEU	3.2
8	D	157	ARG	3.2
6	B	371	SER	3.2
6	B	344	THR	3.2
6	B	711	LEU	3.2
4	4	191	LEU	3.2
1	1	54	PHE	3.1
9	E	85	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
5	A	18	ASP	3.1
4	4	188	SER	3.1
6	B	330	SER	3.1
7	C	44	ARG	3.0
1	1	94	VAL	3.0
2	2	96	PRO	3.0
3	3	105	ASN	3.0
4	4	183	THR	3.0
5	A	25	ASN	3.0
6	B	40	GLU	3.0
5	A	688	SER	3.0
8	D	137	GLN	3.0
7	C	24	ASP	2.9
6	B	500	GLU	2.9
6	B	599	HIS	2.9
2	2	93	SER	2.9
9	E	96	SER	2.9
5	A	382	THR	2.9
5	A	158	GLN	2.9
3	3	136	ALA	2.9
8	D	210	PHE	2.9
6	B	85	VAL	2.9
6	B	287	VAL	2.9
10	F	238	THR	2.9
10	F	98	GLU	2.9
3	3	99	GLY	2.9
5	A	751	GLY	2.9
6	B	396	ILE	2.9
10	F	235	GLU	2.9
6	B	186	VAL	2.8
2	2	160	LEU	2.8
3	3	134	GLY	2.8
6	B	391	GLY	2.8
2	2	145	LYS	2.8
6	B	382	PHE	2.8
4	4	273	SER	2.8
5	A	721	THR	2.8
3	3	85	ASP	2.8
2	2	245	LYS	2.8
6	B	662	PHE	2.8
5	A	566	LYS	2.8
8	D	116	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	2	97	GLU	2.8
3	3	83	GLY	2.8
7	C	65	VAL	2.8
1	1	87	ALA	2.8
5	A	14	LYS	2.7
6	B	357	PRO	2.7
7	C	42	SER	2.7
8	D	115	MET	2.7
11	J	30	ASN	2.7
3	3	77	THR	2.7
8	D	167	LEU	2.7
6	B	650	THR	2.7
5	A	417	TYR	2.7
3	3	142	GLU	2.7
6	B	578	TYR	2.7
6	B	695	LYS	2.7
7	C	49	VAL	2.7
7	C	5	VAL	2.7
7	C	2	ALA	2.7
8	D	87	SER	2.7
1	1	213	PRO	2.6
8	D	93	ARG	2.6
5	A	565	ASP	2.6
5	A	374	MET	2.6
6	B	38	MET	2.6
9	E	97	GLY	2.6
3	3	139	ILE	2.6
6	B	585	LEU	2.6
7	C	3	HIS	2.6
5	A	619	TRP	2.6
4	4	192	VAL	2.6
5	A	583	THR	2.6
5	A	368	ALA	2.6
3	3	272	LEU	2.6
5	A	383	ASP	2.5
6	B	390	HIS	2.5
5	A	632	GLY	2.5
5	A	576	ASP	2.5
8	D	184	GLY	2.5
2	2	125	ILE	2.5
1	1	116	PHE	2.5
5	A	492	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
6	B	684	GLU	2.5
5	A	381	ALA	2.5
6	B	696	ASP	2.5
6	B	587	THR	2.5
6	B	508	SER	2.5
5	A	288	GLY	2.5
2	2	242	ALA	2.5
6	B	10	SER	2.5
6	B	405	LYS	2.4
5	A	738	THR	2.4
6	B	730	THR	2.4
5	A	590	ASP	2.4
5	A	736	ILE	2.4
6	B	517	ASP	2.4
5	A	603	LEU	2.4
5	A	657	VAL	2.4
1	1	147	ASP	2.4
3	3	81	ASP	2.4
6	B	725	PHE	2.4
4	4	272	THR	2.4
5	A	283	ASN	2.4
7	C	74	THR	2.4
10	F	87	GLU	2.4
6	B	58	ILE	2.4
1	1	186	VAL	2.4
1	1	65	LYS	2.4
5	A	557	ALA	2.4
1	1	124	ILE	2.4
5	A	735	GLY	2.4
5	A	686	LEU	2.4
6	B	586	ASN	2.4
6	B	668	TRP	2.4
6	B	654	GLY	2.3
4	4	210	GLN	2.3
5	A	395	MET	2.3
3	3	238	ASN	2.3
6	B	249	ASP	2.3
5	A	265	PHE	2.3
2	2	257	ASP	2.3
8	D	187	GLN	2.3
4	4	327	ILE	2.3
1	1	35	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
6	B	398	ASP	2.3
6	B	305	ILE	2.3
8	D	96	GLN	2.3
5	A	15	ILE	2.3
1	1	162	GLY	2.3
5	A	648	ASP	2.3
6	B	36	ASP	2.3
5	A	559	SER	2.3
4	4	248	ILE	2.3
6	B	142	PHE	2.3
6	B	380	ALA	2.3
6	B	397	ARG	2.3
1	1	109	THR	2.3
7	C	47	ASP	2.3
6	B	631	GLN	2.3
5	A	373	ALA	2.3
6	B	688	LEU	2.3
3	3	227	LYS	2.3
3	3	106	PRO	2.2
5	A	734	GLY	2.2
1	1	206	LEU	2.2
1	1	172	ASP	2.2
3	3	281	ILE	2.2
5	A	255	PRO	2.2
5	A	692	TYR	2.2
6	B	332	HIS	2.2
8	D	131	LYS	2.2
6	B	663	MET	2.2
3	3	138	VAL	2.2
1	1	99	ASN	2.2
11	J	34	PRO	2.2
5	A	597	PHE	2.2
5	A	682	SER	2.2
6	B	584	MET	2.2
4	4	215	LEU	2.2
8	D	186	ASN	2.2
6	B	317	GLY	2.2
6	B	80	THR	2.2
6	B	685	LYS	2.2
6	B	728	ALA	2.2
1	1	208	ASP	2.2
8	D	102	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	3	234	LYS	2.2
8	D	135	LYS	2.2
5	A	296	HIS	2.2
6	B	509	LEU	2.2
2	2	241	HIS	2.2
5	A	601	ASN	2.2
5	A	707	LEU	2.1
8	D	160	ALA	2.1
6	B	81	ASP	2.1
6	B	235	ALA	2.1
6	B	395	PHE	2.1
6	B	664	PHE	2.1
2	2	94	GLU	2.1
5	A	604	SER	2.1
5	A	684	MET	2.1
1	1	184	ALA	2.1
6	B	706	ALA	2.1
8	D	100	PHE	2.1
6	B	385	CYS	2.1
7	C	25	VAL	2.1
8	D	83	ILE	2.1
2	2	238	ALA	2.1
6	B	399	TYR	2.1
7	C	56	THR	2.1
5	A	527	ALA	2.1
8	D	89	GLY	2.1
8	D	161	ASP	2.1
1	1	90	LEU	2.1
6	B	686	THR	2.1
1	1	104	PRO	2.1
6	B	17	PRO	2.1
1	1	183	LEU	2.1
2	2	253	ASP	2.1
5	A	740	TRP	2.1
5	A	542	THR	2.1
11	J	6	THR	2.1
6	B	379	ILE	2.1
6	B	393	ILE	2.1
6	B	675	LEU	2.1
5	A	558	ARG	2.0
4	4	222	LEU	2.0
5	A	698	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	3	249	ALA	2.0
1	1	118	ILE	2.0
6	B	165	SER	2.0
1	1	84	LEU	2.0
3	3	242	ASN	2.0
5	A	582	GLY	2.0
6	B	184	PHE	2.0
6	B	677	GLU	2.0
5	A	241	HIS	2.0
10	F	233	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	DGD	2	811	47/66	0.35	0.40	122,126,134,137	0
20	CAC	3	901	5/5	0.37	0.28	190,190,194,197	0
15	CLA	3	607	50/65	0.38	0.40	195,209,223,228	0
14	BCR	B	4003	40/40	0.49	1.19	125,141,149,153	0
23	GSH	B	5031	20/20	0.51	0.13	151,157,163,166	0
14	BCR	1	505	40/40	0.54	0.63	83,86,98,110	0
23	GSH	4	831	20/20	0.54	0.29	136,138,145,146	0
15	CLA	A	1121	49/65	0.55	0.15	177,193,206,211	0
14	BCR	A	4007	40/40	0.55	0.80	125,132,135,137	0
14	BCR	4	505	40/40	0.56	0.52	83,85,118,119	0
14	BCR	B	4002	40/40	0.56	0.72	114,129,145,146	0
14	BCR	1	503	40/40	0.56	0.85	115,121,136,138	0
15	CLA	3	608	48/65	0.61	0.35	196,222,240,247	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	BCR	J	4003	40/40	0.61	0.38	89,99,105,106	0
12	LUT	3	501	42/42	0.61	0.77	173,180,186,189	0
14	BCR	3	504	40/40	0.62	0.58	137,152,173,173	0
14	BCR	A	4002	40/40	0.62	0.76	120,140,167,169	0
14	BCR	3	503	40/40	0.64	0.66	134,148,166,169	0
15	CLA	A	1131	50/65	0.64	0.34	145,153,157,158	0
18	LMG	2	803	16/55	0.65	0.24	121,129,134,134	0
13	XAT	3	502	44/44	0.65	0.47	154,161,165,166	0
14	BCR	B	4001	40/40	0.65	0.72	121,129,137,138	0
18	LMG	1	803	23/55	0.65	0.30	114,119,150,154	0
21	DGD	J	5001	28/66	0.66	0.52	92,95,97,97	0
18	LMG	1	802	36/55	0.66	0.30	88,102,125,128	0
14	BCR	B	4005	40/40	0.66	0.50	92,95,99,101	0
25	PQN	B	2002	33/33	0.66	0.53	117,129,134,136	0
21	DGD	4	811	45/66	0.66	0.40	83,91,111,119	0
15	CLA	B	1224	49/65	0.67	0.43	106,114,119,121	0
15	CLA	B	1208	49/65	0.67	0.29	131,141,150,152	0
14	BCR	A	4004	40/40	0.67	0.81	136,156,183,186	0
15	CLA	A	1111	49/65	0.68	0.33	122,129,139,142	0
18	LMG	2	802	25/55	0.68	0.33	92,104,127,134	0
15	CLA	B	1203	49/65	0.68	0.40	112,118,123,126	0
15	CLA	B	1023	60/65	0.69	0.40	113,126,138,141	0
14	BCR	A	4003	40/40	0.69	0.54	116,130,150,152	0
14	BCR	4	503	40/40	0.69	0.49	90,93,98,99	0
14	BCR	2	503	40/40	0.70	0.67	96,102,110,110	0
12	LUT	2	501	42/42	0.70	0.53	117,120,125,127	0
15	CLA	3	603	45/65	0.71	0.29	179,187,200,210	0
15	CLA	A	1114	46/65	0.72	0.52	127,141,157,160	0
15	CLA	3	606	45/65	0.73	0.23	156,165,173,177	0
20	CAC	3	902	5/5	0.73	0.26	200,204,206,207	0
15	CLA	B	1022	50/65	0.73	0.38	108,116,124,126	0
15	CLA	B	1215	49/65	0.73	0.41	105,112,119,121	0
15	CLA	B	1238	50/65	0.73	0.32	134,148,155,158	0
16	CHL	3	604	47/66	0.74	0.52	157,171,179,185	0
15	CLA	A	1141	50/65	0.74	0.35	170,186,196,199	0
15	CLA	A	1116	49/65	0.74	0.47	136,151,156,161	0
12	LUT	1	501	42/42	0.74	0.60	100,109,122,125	0
14	BCR	A	4005	40/40	0.74	0.47	129,142,162,163	0
15	CLA	B	1211	49/65	0.75	0.39	127,137,141,143	0
15	CLA	A	1135	49/65	0.75	0.30	126,139,154,160	0
15	CLA	2	605	65/65	0.75	0.26	95,100,104,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	2	602	49/65	0.75	0.25	123,128,133,137	0
25	PQN	A	2001	33/33	0.75	0.47	87,91,98,99	0
15	CLA	B	1221	49/65	0.75	0.37	99,108,113,115	0
15	CLA	B	1218	49/65	0.75	0.24	104,112,117,137	0
15	CLA	1	613	45/65	0.76	0.30	109,119,126,129	0
22	LMT	2	821	23/35	0.77	0.14	109,113,132,138	0
14	BCR	J	4001	40/40	0.77	0.52	83,90,102,103	0
12	LUT	4	501	42/42	0.77	0.44	90,93,101,102	0
15	CLA	A	1126	49/65	0.77	0.42	98,106,108,108	0
15	CLA	4	607	49/65	0.77	0.23	92,98,104,105	0
15	CLA	A	1108	46/65	0.78	0.32	123,132,140,143	0
20	CAC	4	902	5/5	0.78	0.23	85,105,119,122	0
15	CLA	A	1134	49/65	0.78	0.22	162,171,183,186	0
15	CLA	2	606	46/65	0.78	0.43	105,111,116,119	0
15	CLA	3	601	49/65	0.78	0.27	165,175,188,190	0
15	CLA	3	612	55/65	0.79	0.34	135,143,151,153	0
14	BCR	J	4002	40/40	0.79	0.35	88,91,99,100	0
15	CLA	B	1236	49/65	0.79	0.34	83,87,90,90	0
14	BCR	A	4006	40/40	0.79	0.38	83,91,102,103	0
15	CLA	A	1117	49/65	0.79	0.35	132,136,143,147	0
15	CLA	B	1226	49/65	0.79	0.29	105,112,118,120	0
15	CLA	1	601	49/65	0.79	0.31	111,114,118,119	0
15	CLA	B	1219	49/65	0.79	0.34	95,103,107,108	0
16	CHL	1	610	47/66	0.79	0.27	101,105,111,114	0
15	CLA	A	1124	49/65	0.79	0.31	123,133,142,148	0
15	CLA	4	615	55/65	0.79	0.32	82,84,86,87	0
15	CLA	3	611	46/65	0.79	0.34	147,154,162,167	0
21	DGD	B	5002	38/66	0.79	0.29	114,119,125,127	0
15	CLA	1	615	65/65	0.79	0.38	83,85,89,91	0
14	BCR	B	4006	40/40	0.80	0.65	80,83,89,90	0
15	CLA	A	1120	49/65	0.80	0.26	162,176,190,191	0
15	CLA	2	612	49/65	0.81	0.28	91,97,100,102	0
15	CLA	3	613	46/65	0.81	0.36	150,153,186,194	0
17	LHG	2	801	21/49	0.81	0.25	121,128,134,137	0
15	CLA	A	1128	49/65	0.81	0.34	102,113,116,117	0
15	CLA	A	1119	49/65	0.81	0.35	140,151,159,162	0
15	CLA	B	1021	65/65	0.81	0.33	89,103,107,108	0
15	CLA	B	1212	45/65	0.81	0.28	128,138,147,148	0
13	XAT	4	502	44/44	0.81	0.33	83,84,88,89	0
15	CLA	4	606	49/65	0.81	0.63	89,94,97,98	0
15	CLA	A	1137	49/65	0.82	0.31	137,144,151,153	0
15	CLA	A	1123	48/65	0.82	0.31	128,139,146,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	A	1136	49/65	0.82	0.24	140,148,154,159	0
15	CLA	2	601	49/65	0.82	0.26	110,116,125,129	0
15	CLA	A	1113	45/65	0.82	0.36	147,155,160,161	0
15	CLA	A	1118	49/65	0.82	0.32	151,164,172,175	0
15	CLA	2	604	49/65	0.82	0.20	104,111,117,119	0
20	CAC	1	902	5/5	0.82	0.23	136,142,150,152	0
14	BCR	F	4002	40/40	0.82	0.37	80,81,81,82	0
15	CLA	B	1213	49/65	0.82	0.26	111,117,123,125	0
15	CLA	F	1302	49/65	0.82	0.23	81,83,86,86	0
15	CLA	B	1207	25/65	0.82	0.30	145,151,156,158	0
15	CLA	1	607	46/65	0.82	0.32	99,104,109,111	0
15	CLA	B	1220	55/65	0.82	0.26	91,98,102,103	0
19	SQD	1	811	40/54	0.82	0.21	100,104,109,109	0
15	CLA	3	610	49/65	0.82	0.29	134,143,160,173	0
15	CLA	A	1133	49/65	0.83	0.28	147,157,165,169	0
15	CLA	A	1101	45/65	0.83	0.33	90,95,99,100	0
16	CHL	4	613	50/66	0.83	0.44	86,91,96,98	0
13	XAT	1	502	44/44	0.83	0.59	89,97,109,110	0
15	CLA	1	603	45/65	0.83	0.28	91,95,97,99	0
17	LHG	A	5001	16/49	0.83	0.20	165,168,172,175	0
13	XAT	2	502	44/44	0.83	0.36	103,107,110,110	0
15	CLA	1	605	48/65	0.83	0.39	93,97,101,103	0
15	CLA	B	1232	49/65	0.83	0.28	92,99,103,105	0
15	CLA	A	1140	55/65	0.84	0.34	89,93,98,100	0
15	CLA	A	1109	49/65	0.84	0.17	103,111,114,115	0
15	CLA	B	1205	49/65	0.84	0.26	122,126,132,134	0
15	CLA	1	612	60/65	0.84	0.28	97,105,110,112	0
15	CLA	A	1112	49/65	0.84	0.39	124,131,141,144	0
15	CLA	2	615	50/65	0.84	0.26	112,124,141,146	0
15	CLA	B	1225	49/65	0.84	0.33	108,114,122,126	0
15	CLA	A	1132	49/65	0.84	0.45	137,148,163,168	0
15	CLA	A	1104	60/65	0.85	0.40	103,109,115,118	0
15	CLA	B	1239	65/65	0.85	0.28	120,125,155,163	0
15	CLA	4	612	49/65	0.85	0.20	81,84,85,86	0
15	CLA	1	611	49/65	0.85	0.21	110,118,124,126	0
14	BCR	B	4004	40/40	0.85	0.30	92,94,97,98	0
15	CLA	B	1201	49/65	0.85	0.25	127,132,139,152	0
15	CLA	A	1130	55/65	0.85	0.29	157,163,172,174	0
15	CLA	B	1240	65/65	0.85	0.26	84,92,97,99	0
15	CLA	A	1127	49/65	0.85	0.34	109,118,123,125	0
24	CL0	A	1011	50/65	0.85	0.35	100,104,112,115	0
15	CLA	1	602	46/65	0.85	0.31	106,110,115,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	B	1223	50/65	0.85	0.34	91,97,99,101	0
15	CLA	B	1230	49/65	0.86	0.30	81,83,85,86	0
15	CLA	A	1013	65/65	0.86	0.32	86,90,97,99	0
15	CLA	B	1237	49/65	0.86	0.17	140,150,158,161	0
15	CLA	B	1214	49/65	0.86	0.35	102,105,111,112	0
17	LHG	1	801	23/49	0.86	0.28	95,99,101,103	0
16	CHL	4	610	47/66	0.86	0.27	82,85,87,87	0
15	CLA	2	608	49/65	0.86	0.35	128,136,143,146	0
15	CLA	B	1229	65/65	0.86	0.37	80,81,82,83	0
15	CLA	B	1227	45/65	0.86	0.20	85,88,91,92	0
15	CLA	2	607	49/65	0.86	0.37	125,132,139,141	0
15	CLA	A	1125	49/65	0.86	0.29	137,141,146,148	0
15	CLA	1	604	49/65	0.87	0.24	93,95,97,98	0
15	CLA	B	1228	60/65	0.87	0.31	79,82,84,85	0
15	CLA	A	1012	60/65	0.87	0.39	89,92,98,100	0
15	CLA	1	606	45/65	0.87	0.22	110,116,120,122	0
15	CLA	A	1110	49/65	0.87	0.22	140,149,157,161	0
15	CLA	A	1122	49/65	0.87	0.26	144,154,161,164	0
15	CLA	3	615	46/65	0.87	0.27	118,127,131,133	0
15	CLA	B	1216	49/65	0.87	0.22	97,105,108,108	0
15	CLA	B	1206	49/65	0.88	0.28	131,139,145,148	0
17	LHG	A	5002	24/49	0.88	0.35	99,105,107,108	0
15	CLA	4	602	49/65	0.88	0.27	95,99,104,107	0
16	CHL	2	611	48/66	0.88	0.25	103,104,111,114	0
15	CLA	A	1129	48/65	0.88	0.28	147,160,175,178	0
15	CLA	F	1301	47/65	0.88	0.24	81,82,83,85	0
15	CLA	B	1202	49/65	0.88	0.29	111,117,121,125	0
16	CHL	2	613	46/66	0.88	0.30	100,102,103,105	0
16	CHL	2	609	50/66	0.88	0.20	119,129,136,138	0
15	CLA	A	1102	45/65	0.88	0.27	100,106,109,111	0
16	CHL	2	610	50/66	0.88	0.16	97,100,102,103	0
15	CLA	A	1103	55/65	0.88	0.31	111,121,125,128	0
15	CLA	4	604	49/65	0.88	0.22	82,86,89,89	0
15	CLA	A	1115	49/65	0.88	0.40	160,166,178,179	0
15	CLA	2	603	46/65	0.89	0.23	115,122,128,129	0
15	CLA	J	1302	49/65	0.89	0.24	86,89,91,92	0
15	CLA	A	1107	49/65	0.89	0.31	85,91,94,96	0
20	CAC	1	901	5/5	0.89	0.21	130,132,142,147	0
17	LHG	B	5001	21/49	0.89	0.20	88,89,92,93	0
15	CLA	A	1106	65/65	0.89	0.33	89,98,104,105	0
15	CLA	B	1234	49/65	0.89	0.25	86,91,94,95	0
15	CLA	4	609	49/65	0.89	0.29	87,92,96,97	0

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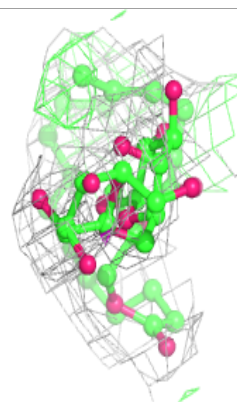
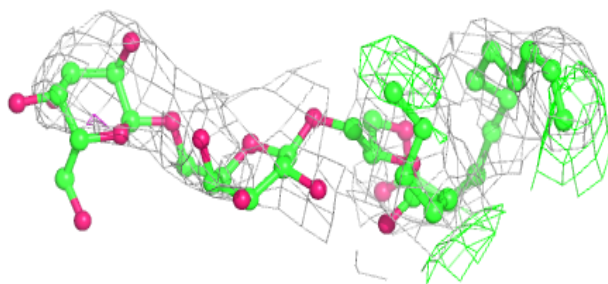
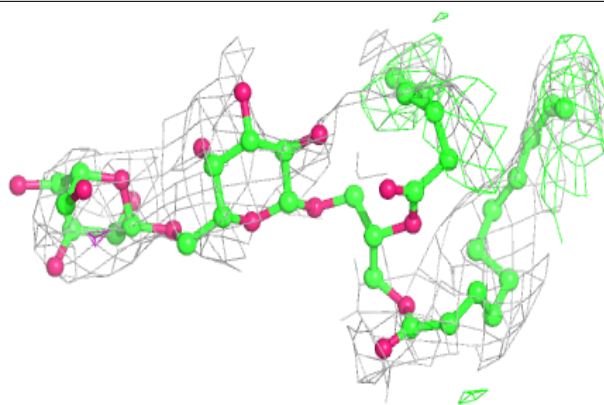
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CLA	4	601	49/65	0.90	0.24	92,95,100,101	0
15	CLA	A	1139	52/65	0.90	0.28	85,88,91,92	0
15	CLA	4	608	46/65	0.90	0.20	92,96,101,103	0
15	CLA	A	1105	49/65	0.90	0.19	94,98,104,105	0
15	CLA	1	608	46/65	0.90	0.45	91,96,101,103	0
15	CLA	B	1209	46/65	0.90	0.17	130,133,140,141	0
15	CLA	B	1231	60/65	0.90	0.26	88,95,99,101	0
15	CLA	3	605	46/65	0.90	0.25	142,151,156,159	0
15	CLA	4	603	49/65	0.90	0.19	85,89,92,93	0
16	CHL	4	611	50/66	0.90	0.22	88,92,96,99	0
15	CLA	4	605	49/65	0.91	0.19	80,82,83,84	0
15	CLA	B	1210	49/65	0.91	0.21	116,124,127,128	0
15	CLA	B	1235	60/65	0.91	0.22	80,83,86,87	0
15	CLA	B	1204	49/65	0.91	0.18	134,146,151,153	0
16	CHL	1	609	50/66	0.92	0.29	88,91,96,97	0
20	CAC	4	901	5/5	0.92	0.21	133,136,139,139	0
15	CLA	A	1138	65/65	0.92	0.39	82,84,86,87	0
15	CLA	B	1217	46/65	0.92	0.18	121,128,132,134	0
15	CLA	B	1222	49/65	0.93	0.29	87,93,96,96	0
27	CA	B	6000	1/1	0.94	0.17	97,97,97,97	0
26	SF4	C	3002	8/8	0.96	0.16	121,123,127,198	0
26	SF4	C	3003	8/8	0.97	0.11	115,117,119,120	0
26	SF4	A	3001	8/8	0.98	0.23	108,110,111,113	0

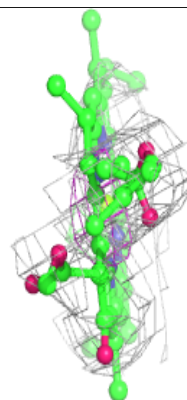
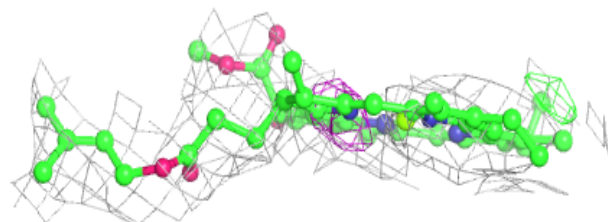
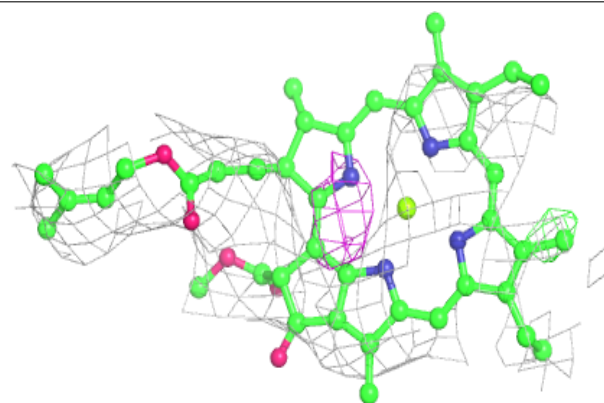
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DGD 2 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

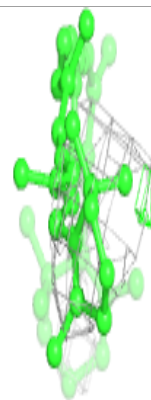
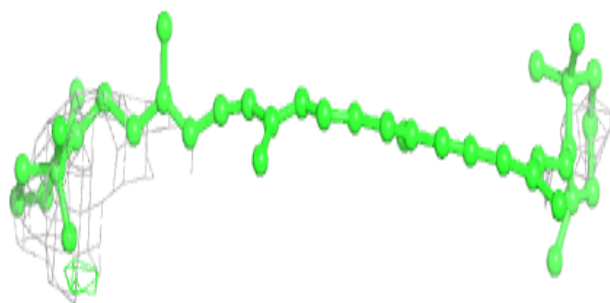
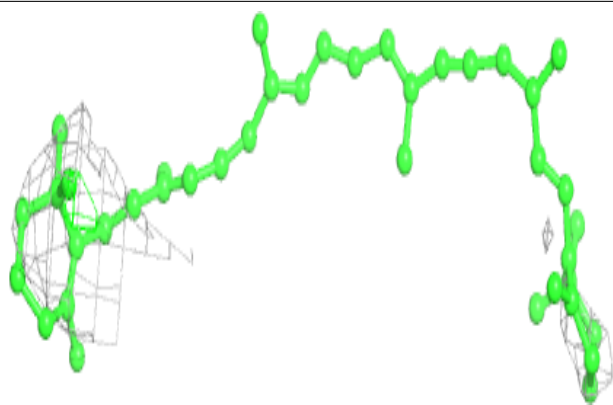
**Electron density around CLA 3 607:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



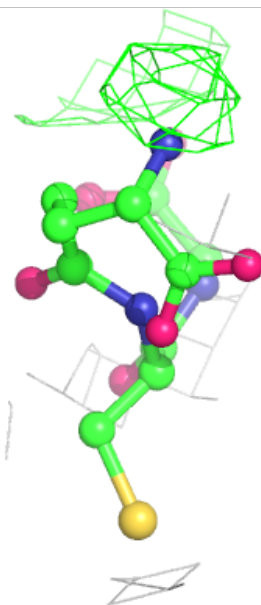
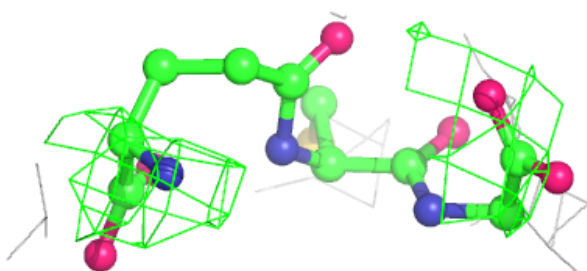
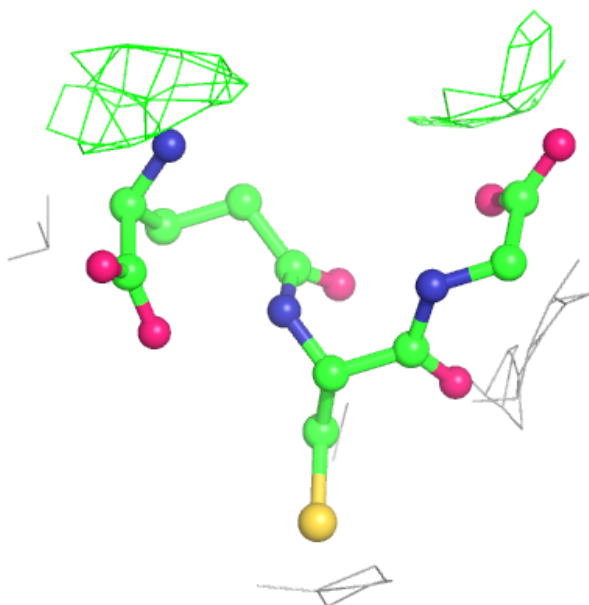
Electron density around BCR B 4003:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



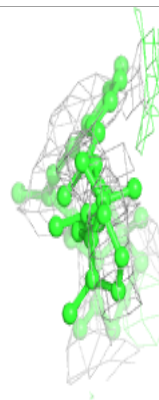
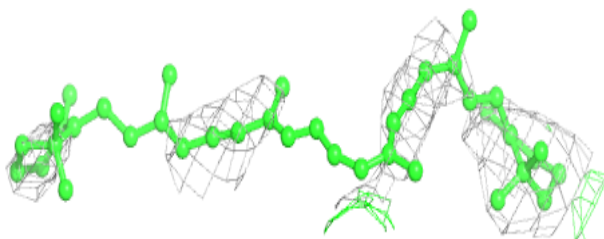
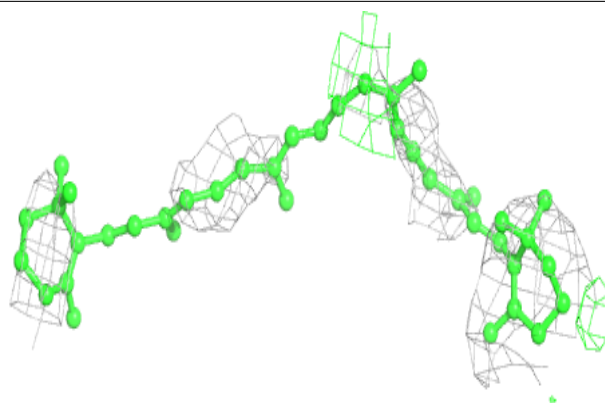
Electron density around GSH B 5031:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

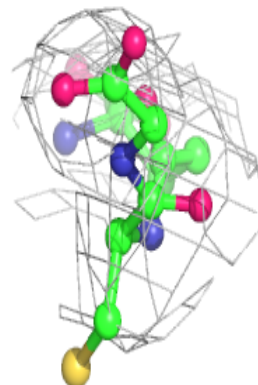
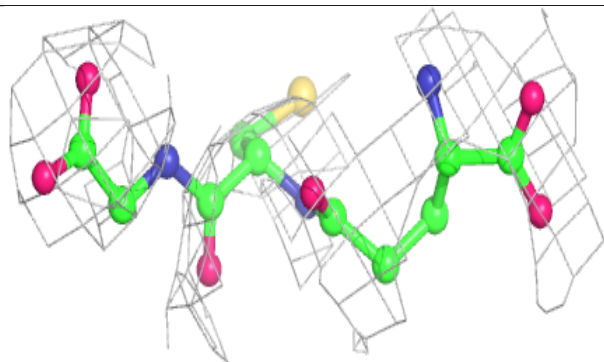
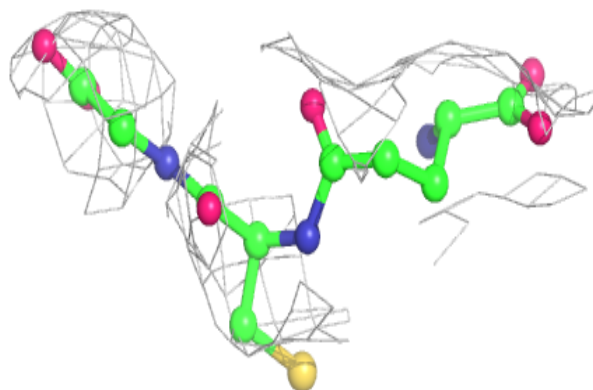


Electron density around BCR 1 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

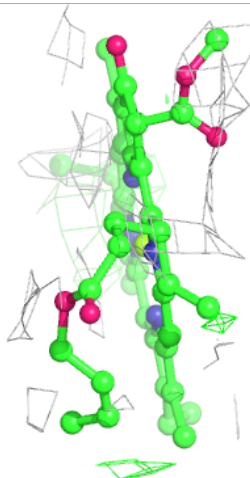
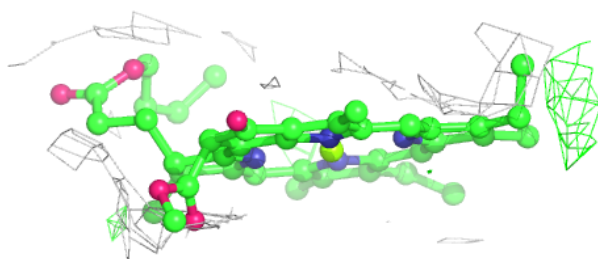
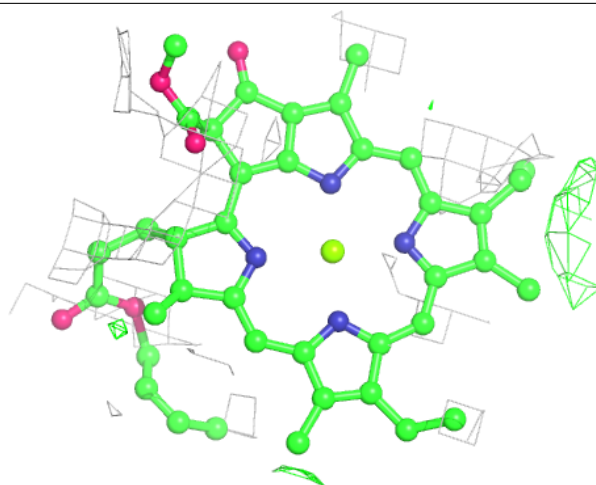
**Electron density around GSH 4 831:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



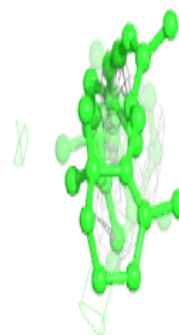
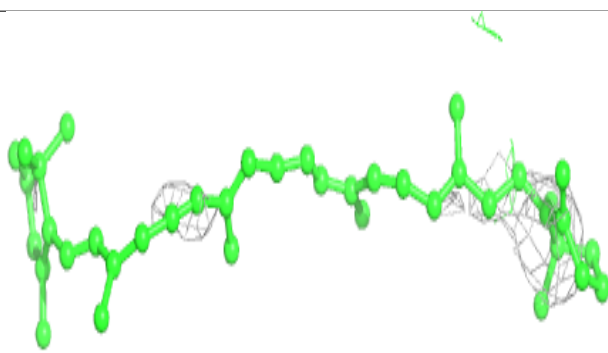
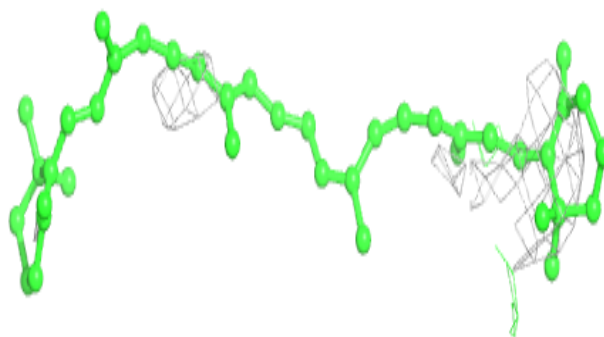
Electron density around CLA A 1121:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

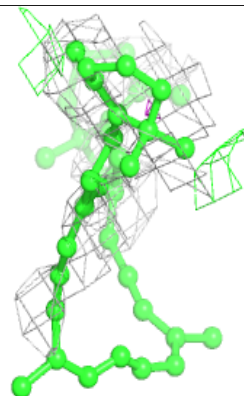
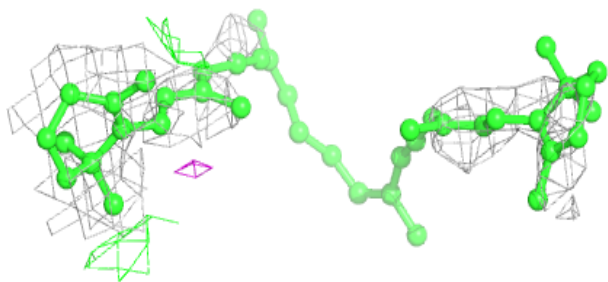
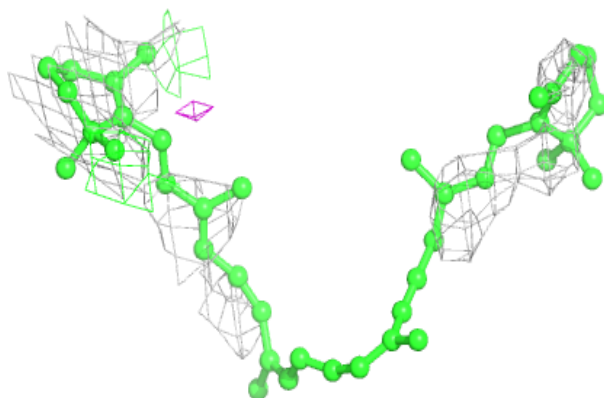


Electron density around BCR A 4007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

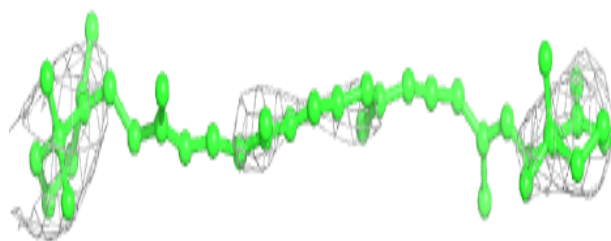
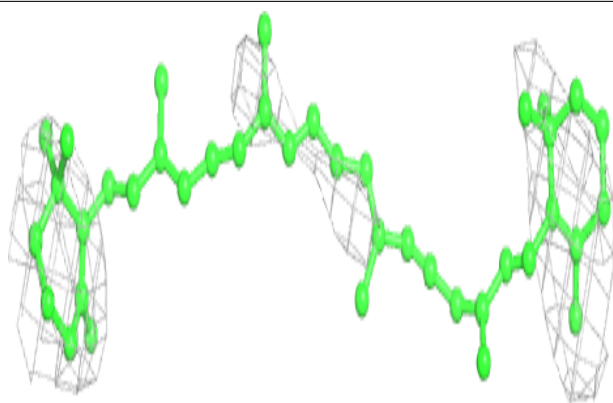
**Electron density around BCR 4 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

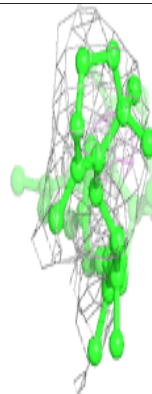
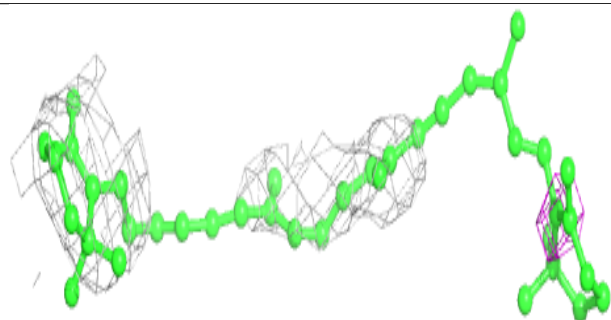
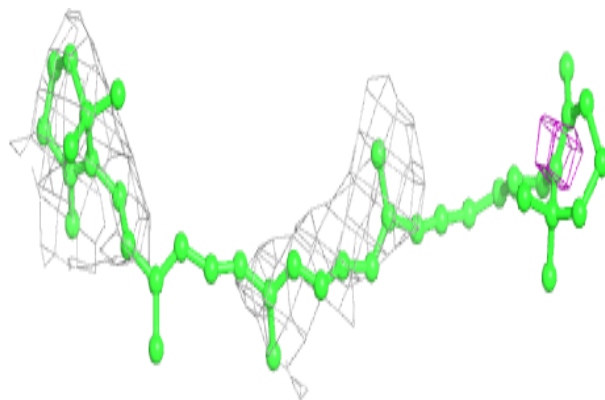


Electron density around BCR B 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

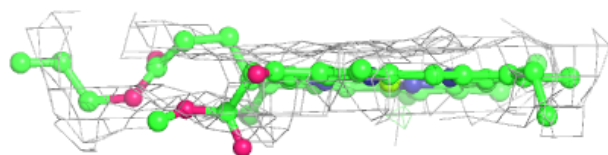
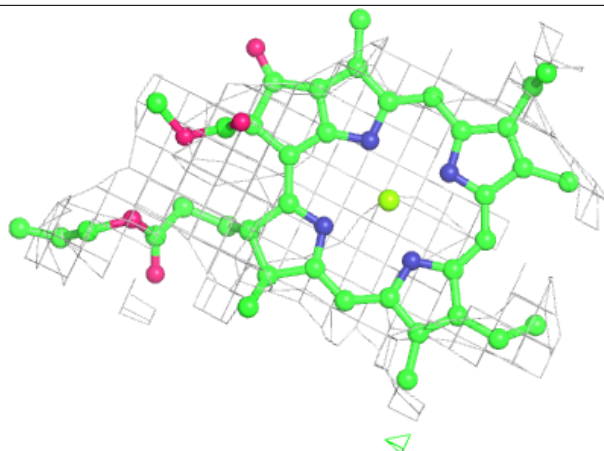
**Electron density around BCR 1 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

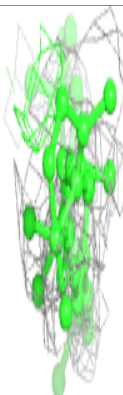
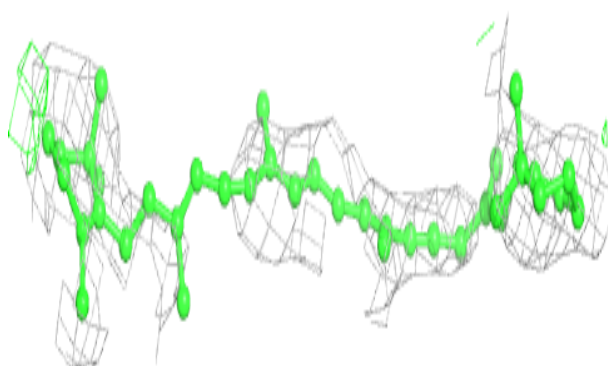
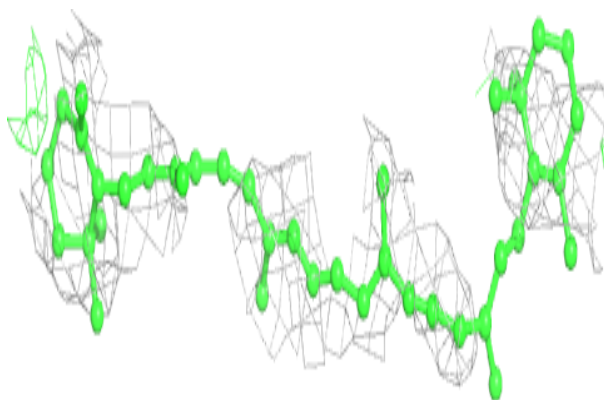


Electron density around CLA 3 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

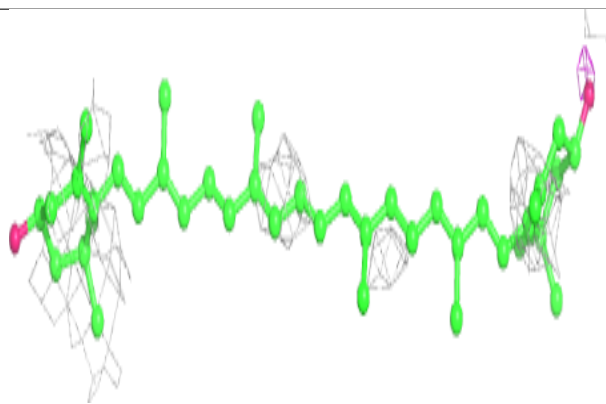
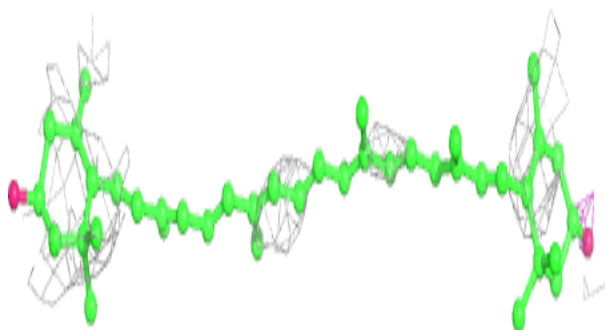
**Electron density around BCR J 4003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

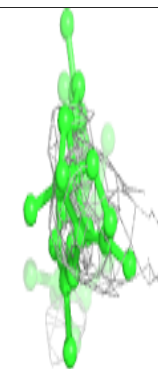
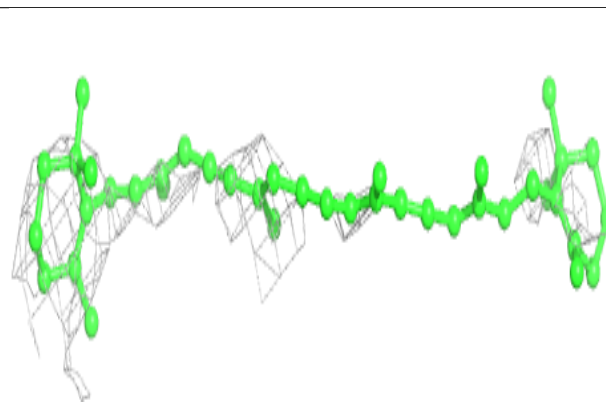
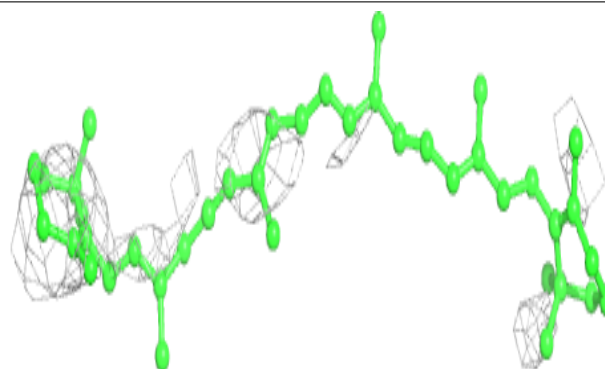


Electron density around LUT 3 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

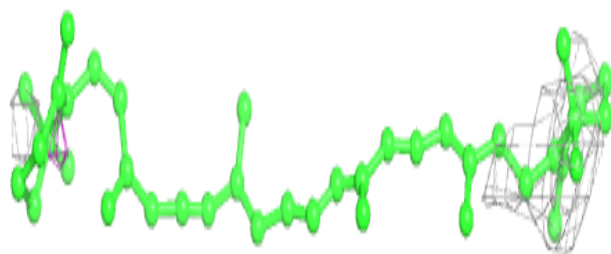
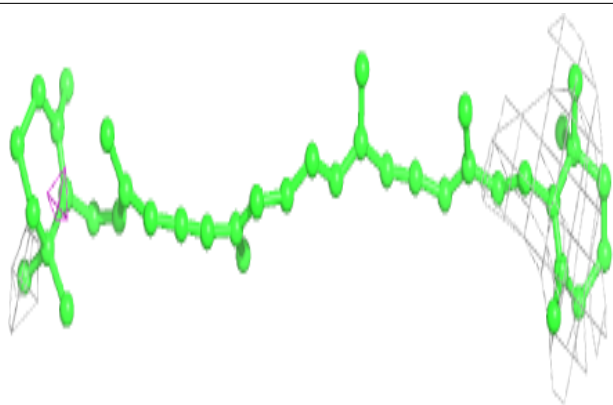
**Electron density around BCR 3 504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

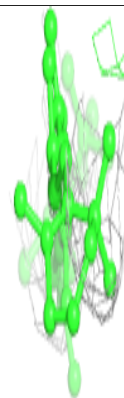
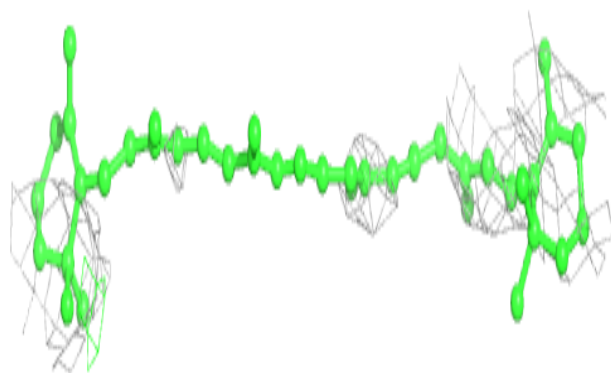
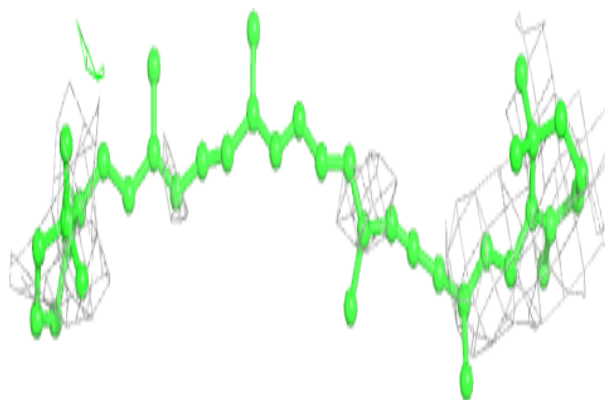


Electron density around BCR A 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

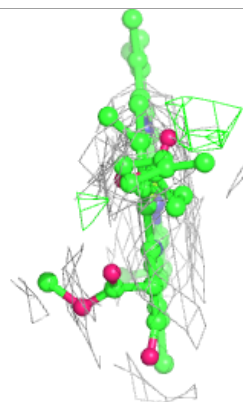
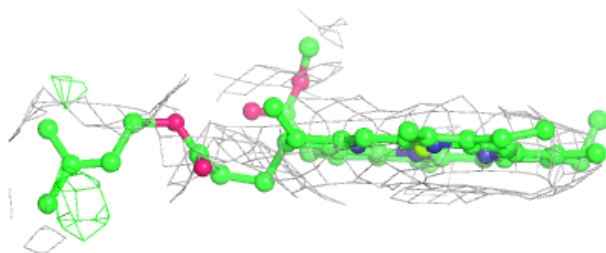
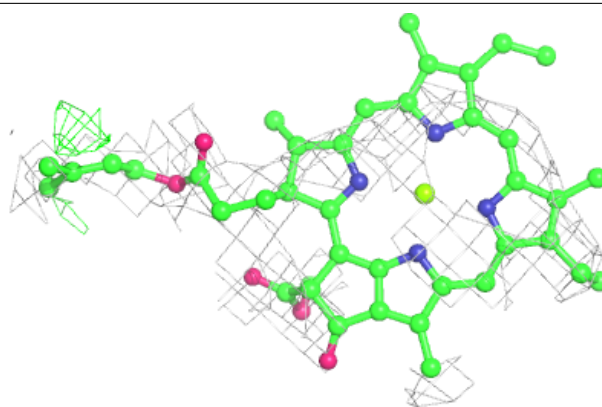
**Electron density around BCR 3 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

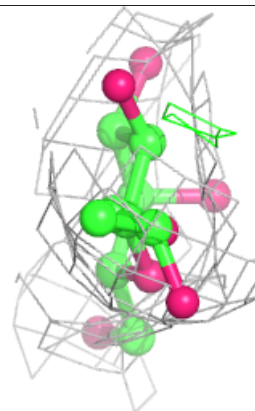
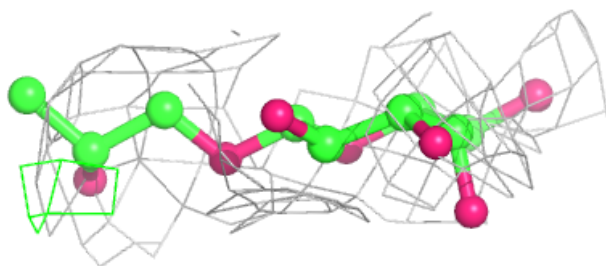
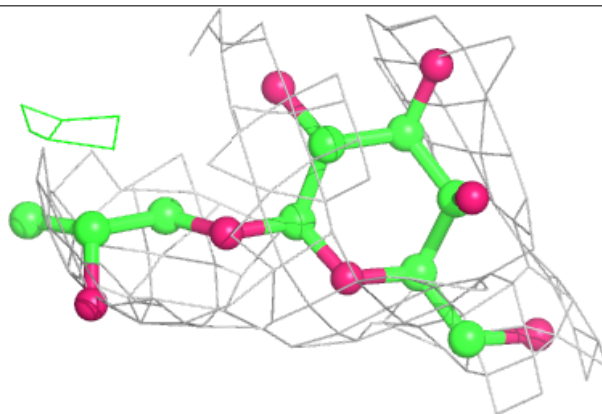


Electron density around CLA A 1131:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

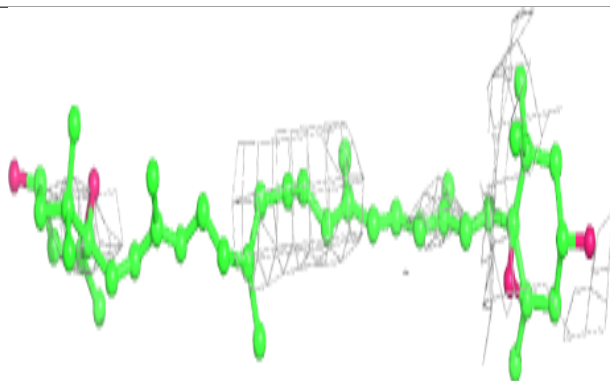
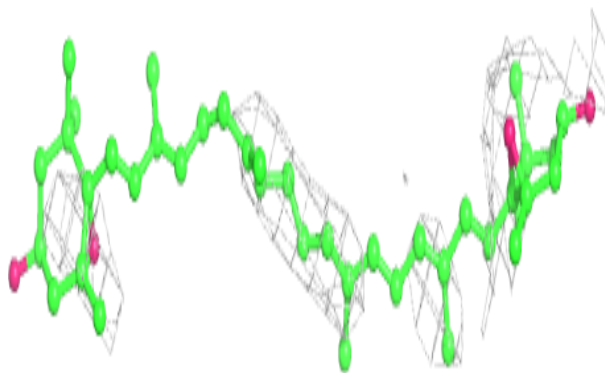
**Electron density around LMG 2 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

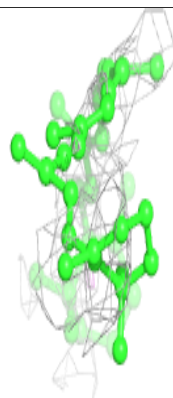
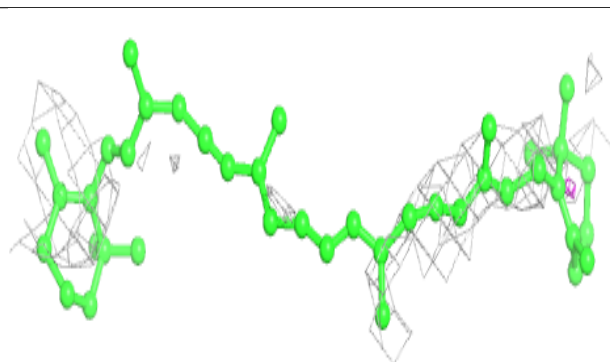
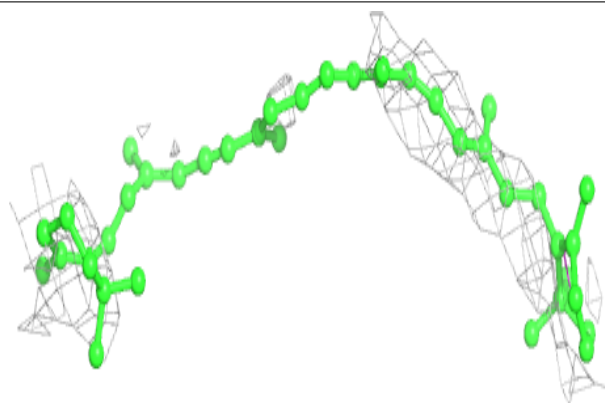


Electron density around XAT 3 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

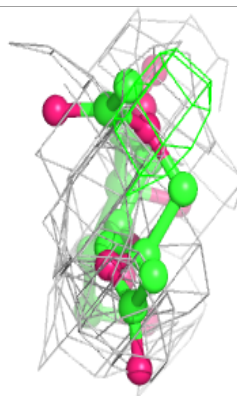
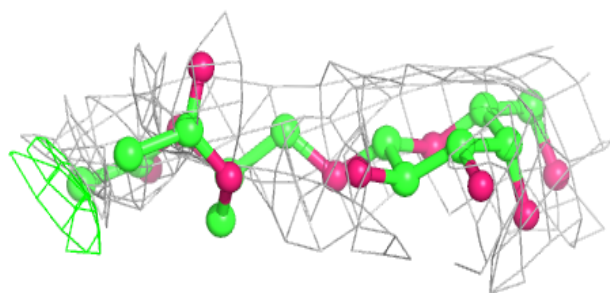
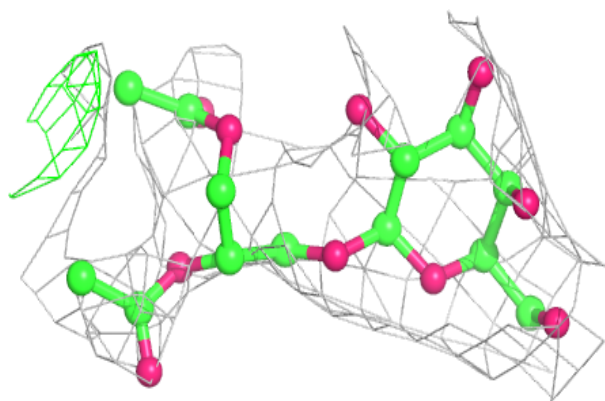
**Electron density around BCR B 4001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

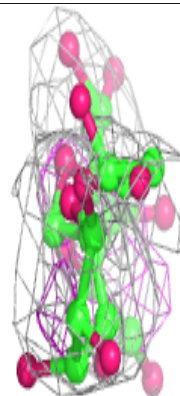
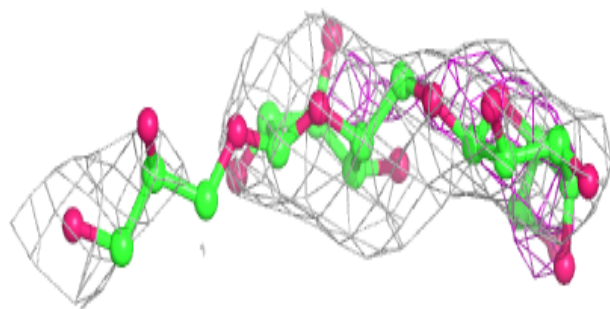
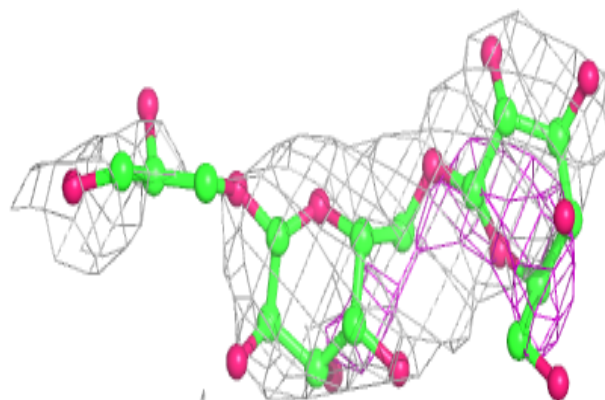


Electron density around LMG 1 803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

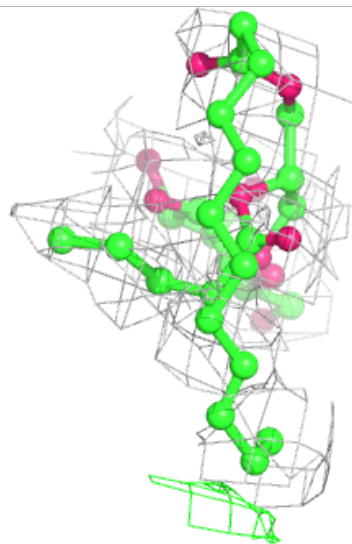
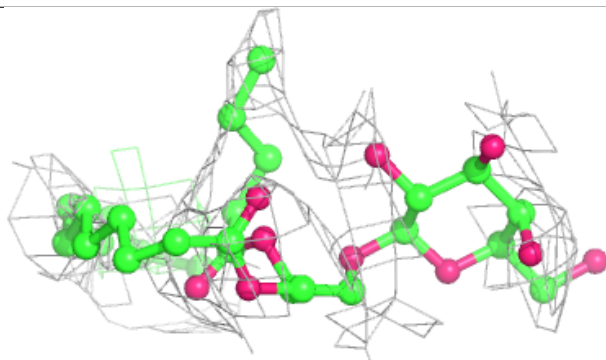
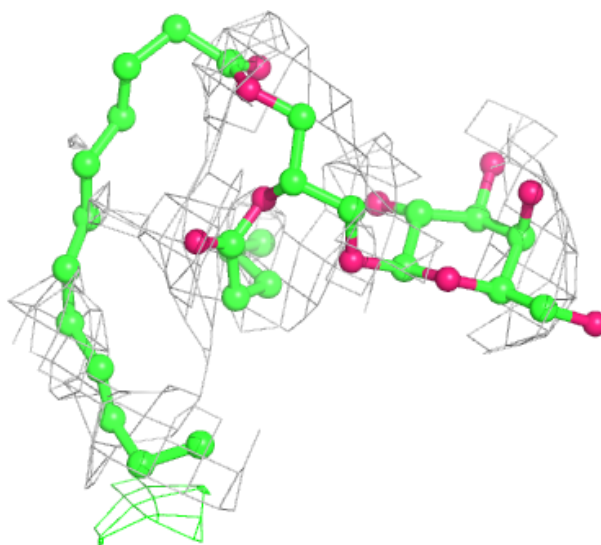
**Electron density around DGD J 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



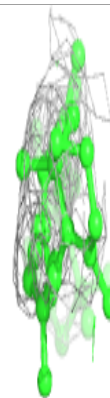
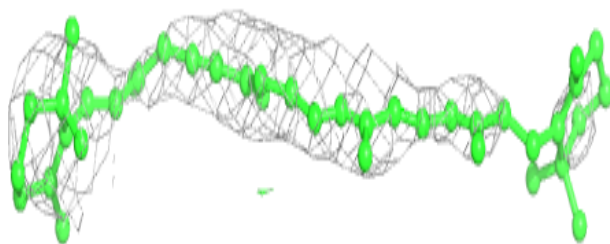
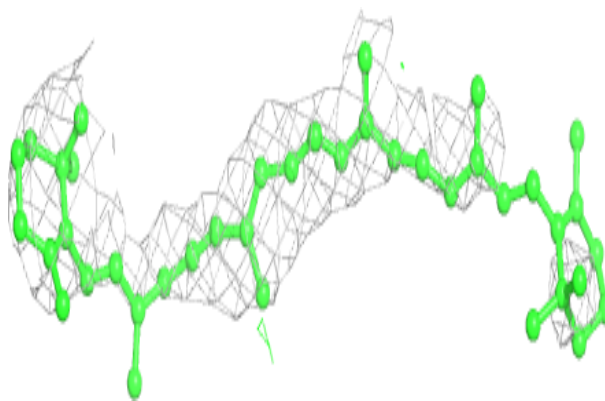
Electron density around LMG 1 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

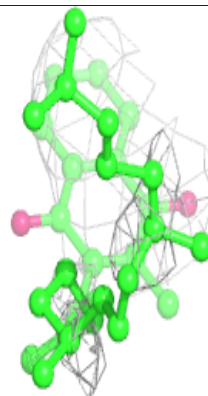
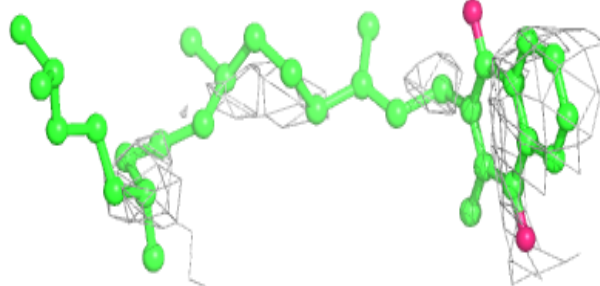
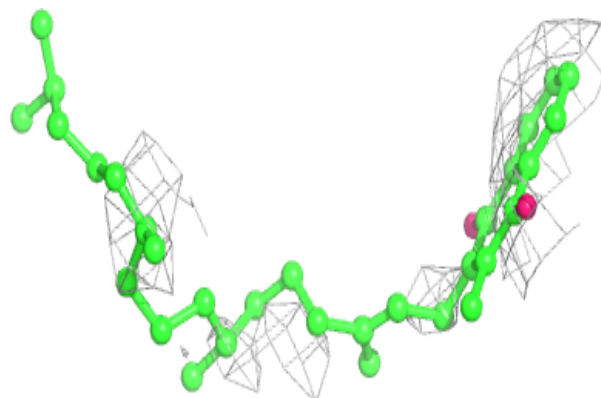


Electron density around BCR B 4005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

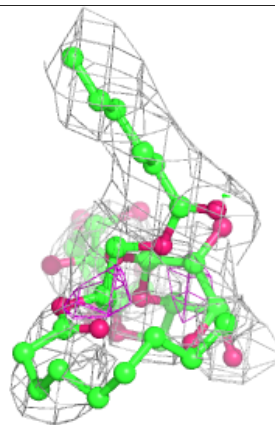
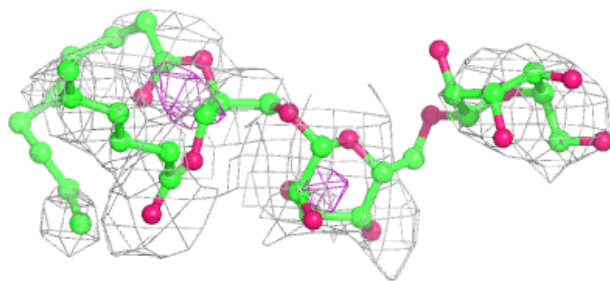
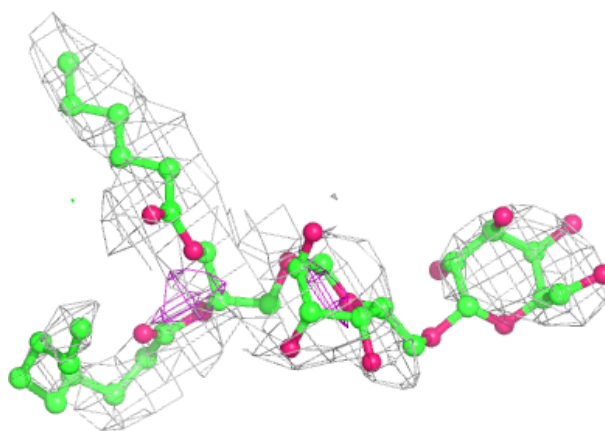
**Electron density around PQN B 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



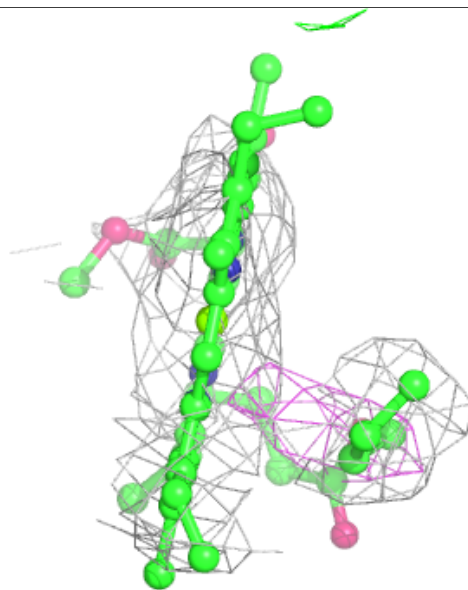
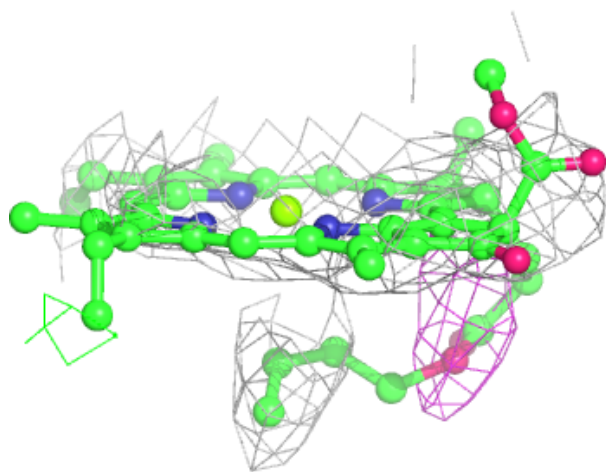
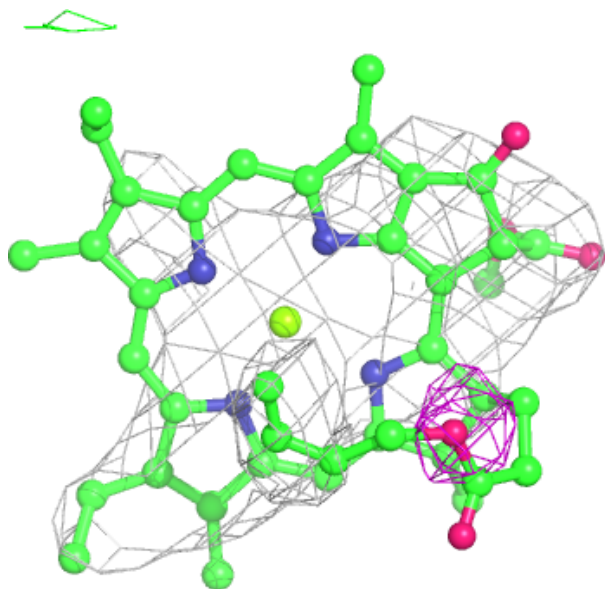
Electron density around DGD 4 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



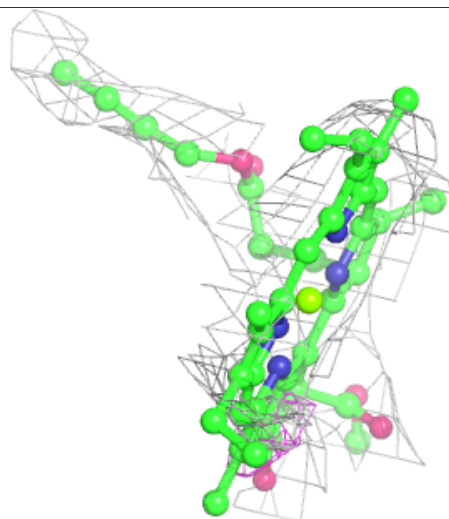
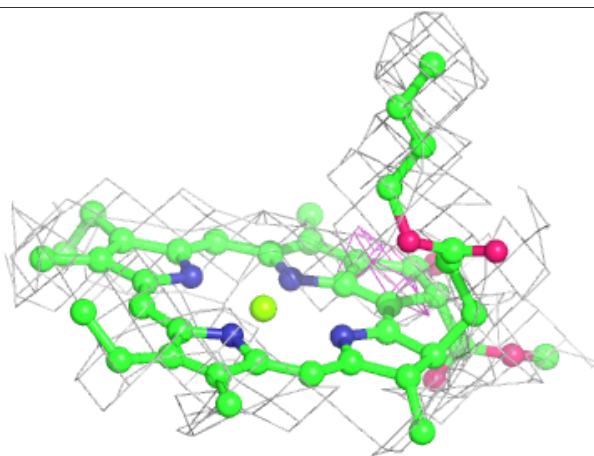
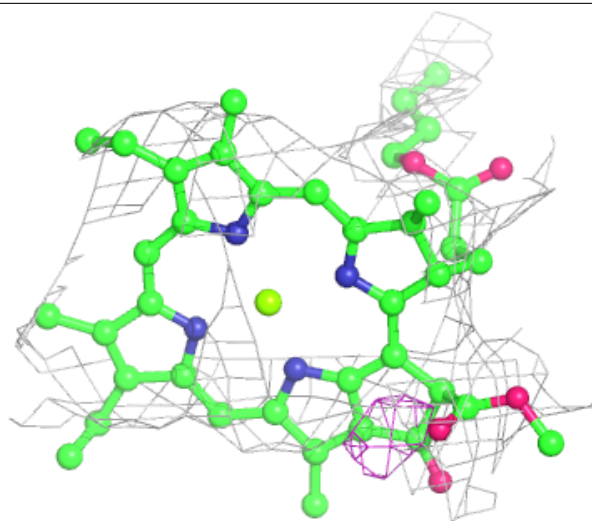
Electron density around CLA B 1224:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



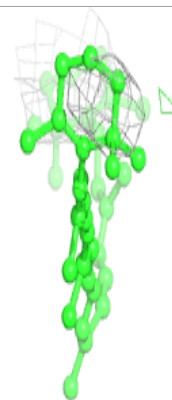
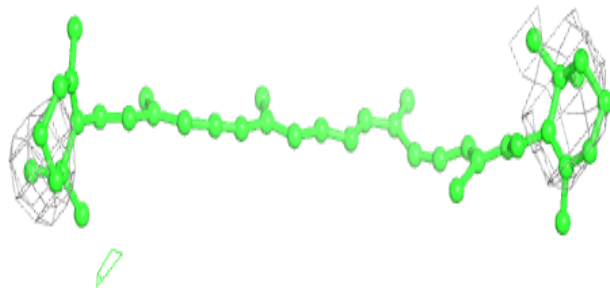
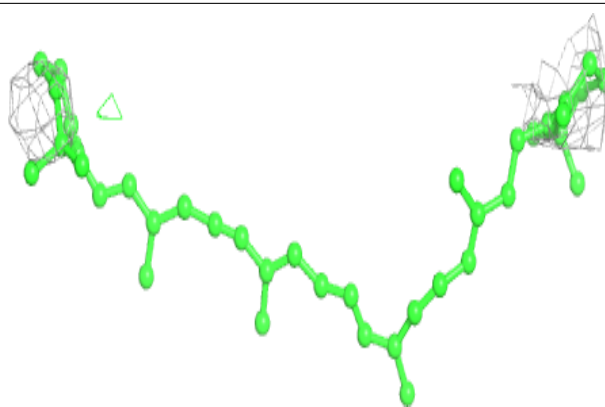
Electron density around CLA B 1208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



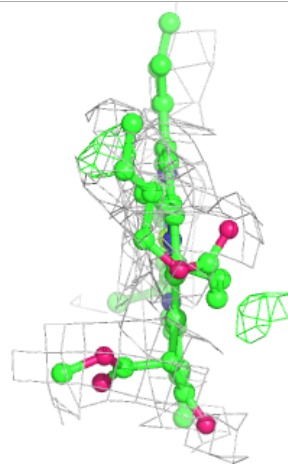
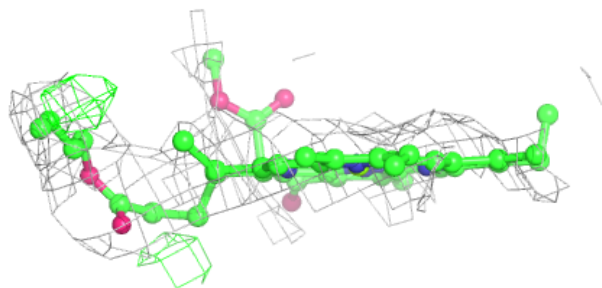
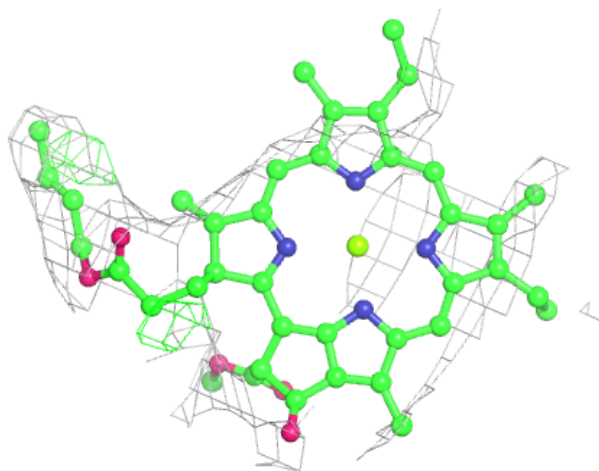
Electron density around BCR A 4004:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



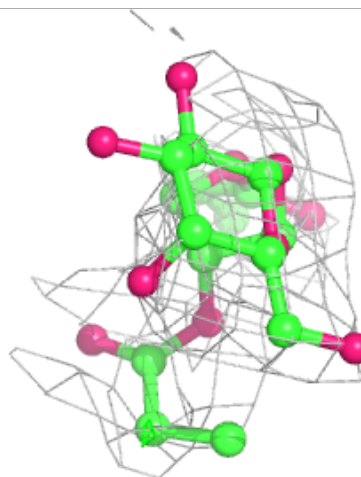
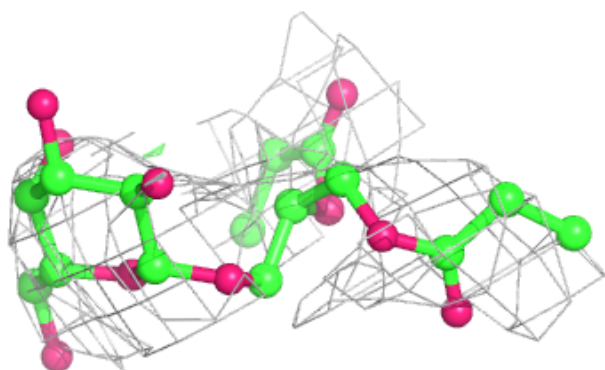
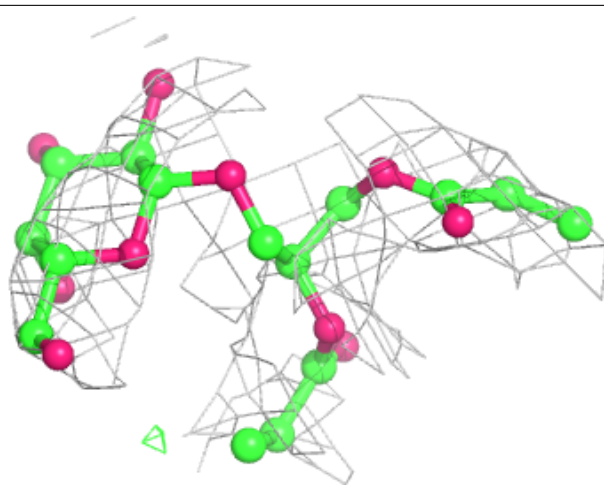
Electron density around CLA A 1111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



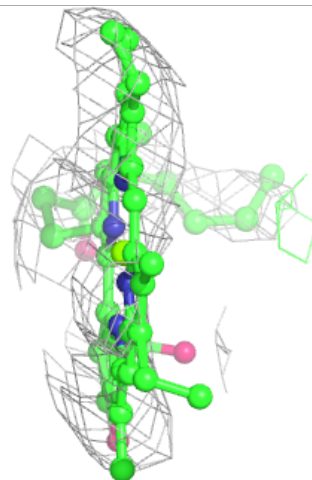
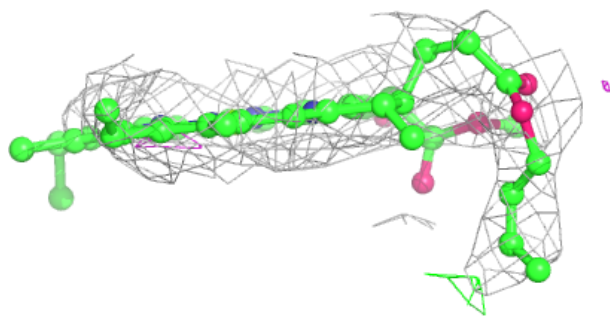
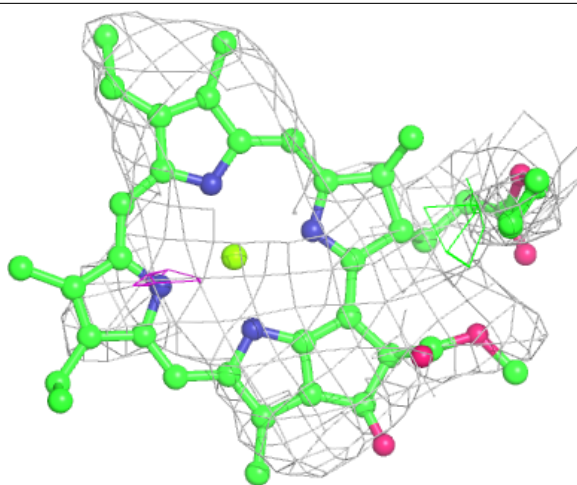
Electron density around LMG 2 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



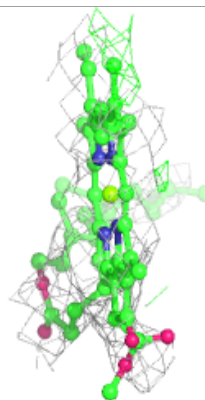
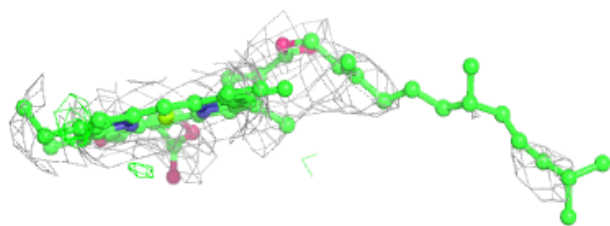
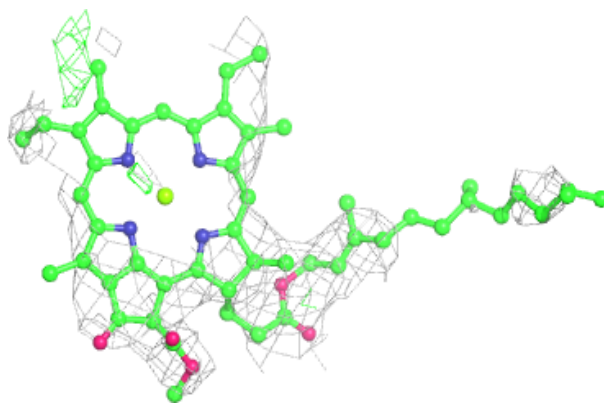
Electron density around CLA B 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

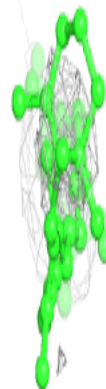
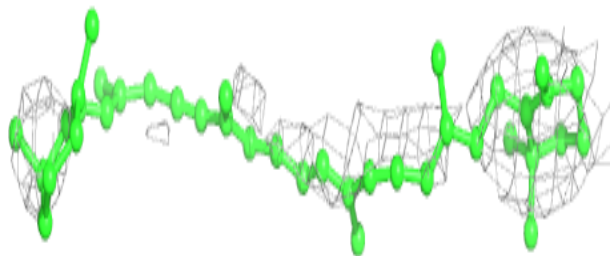
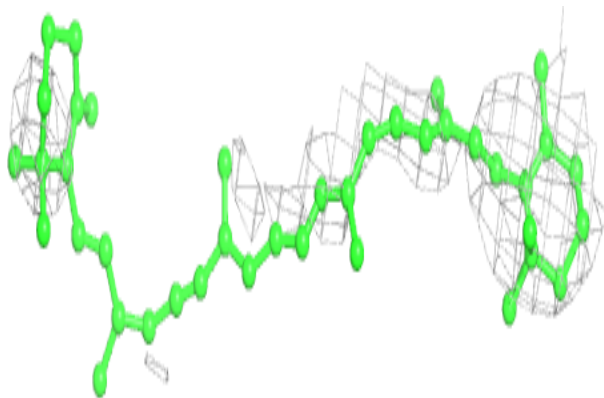


Electron density around CLA B 1023:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

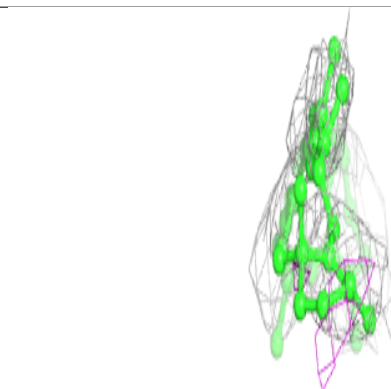
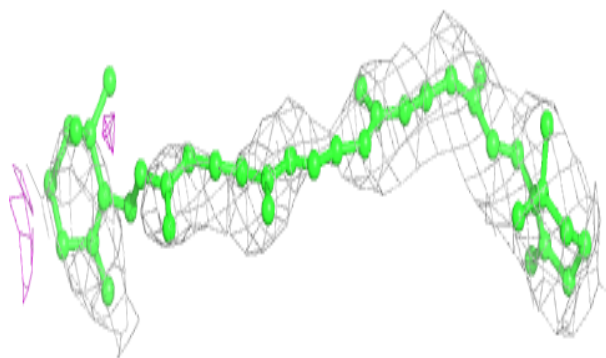
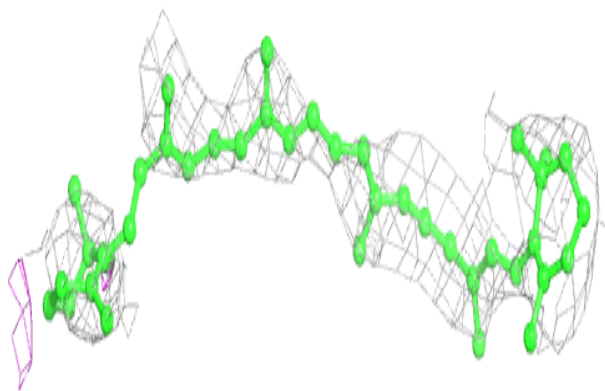
**Electron density around BCR A 4003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

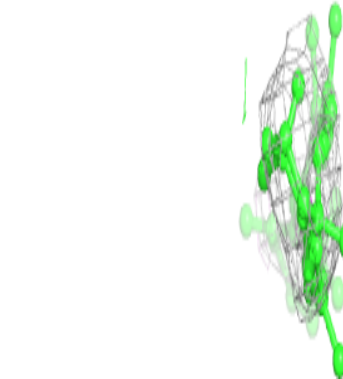
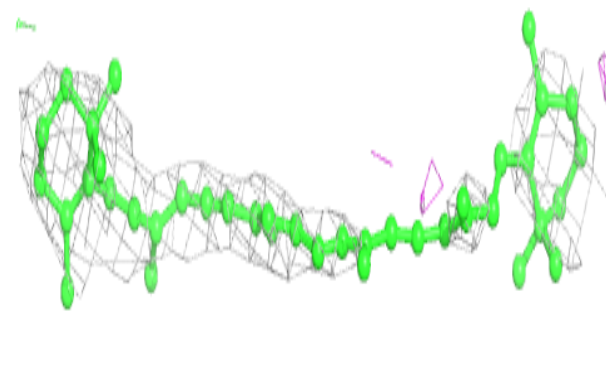
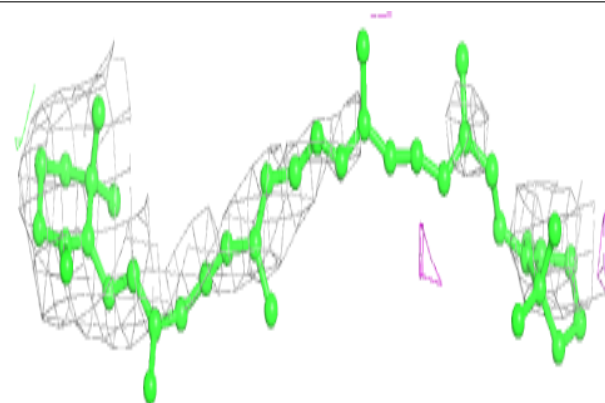


Electron density around BCR 4 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

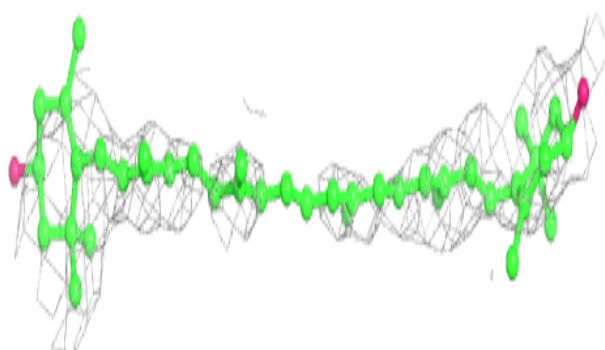
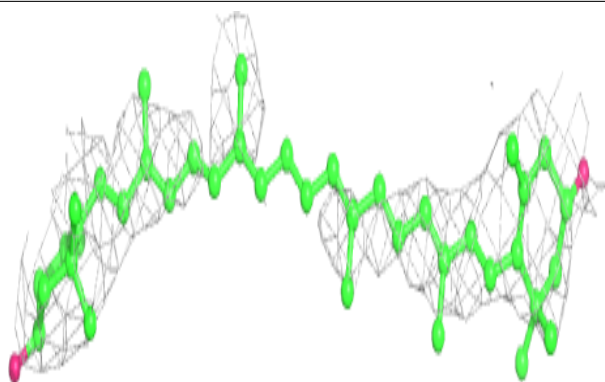
**Electron density around BCR 2 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



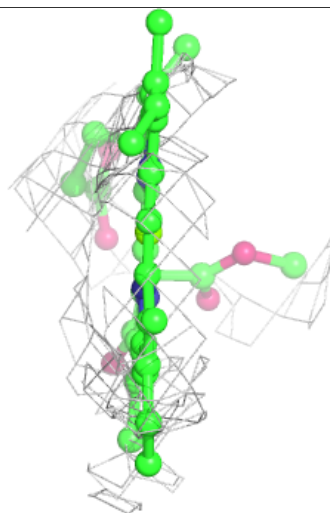
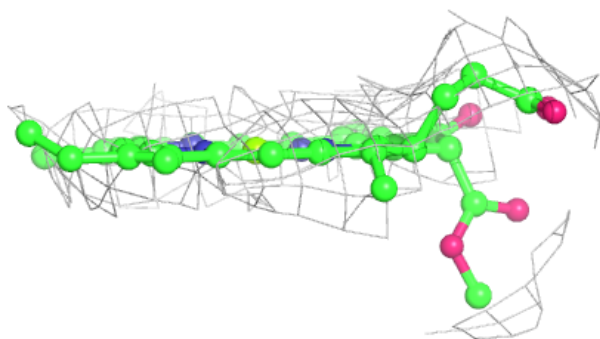
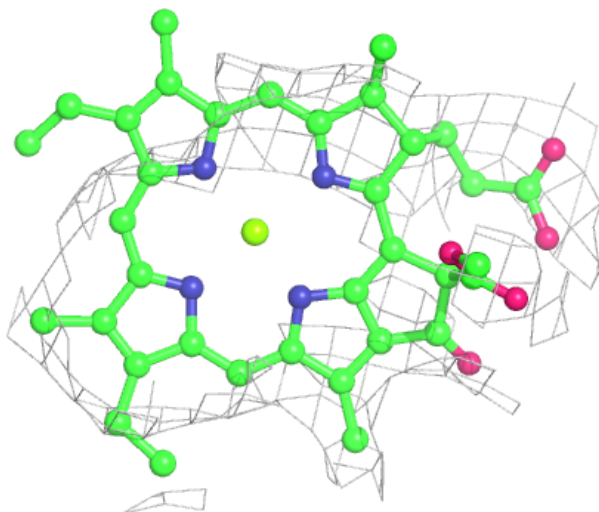
Electron density around LUT 2 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



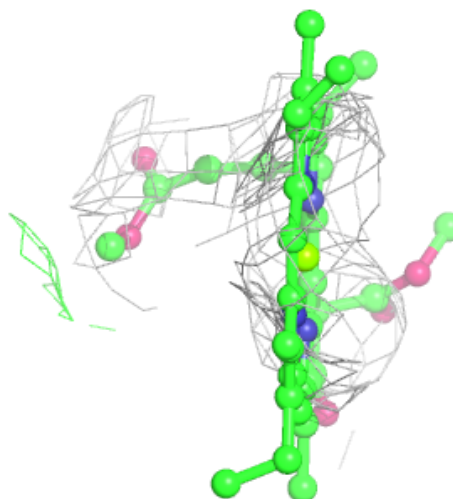
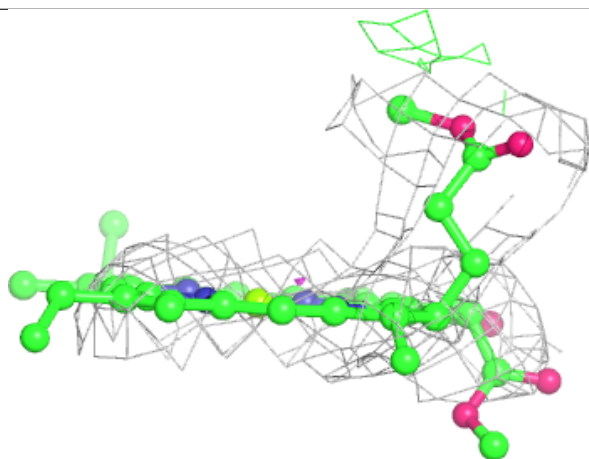
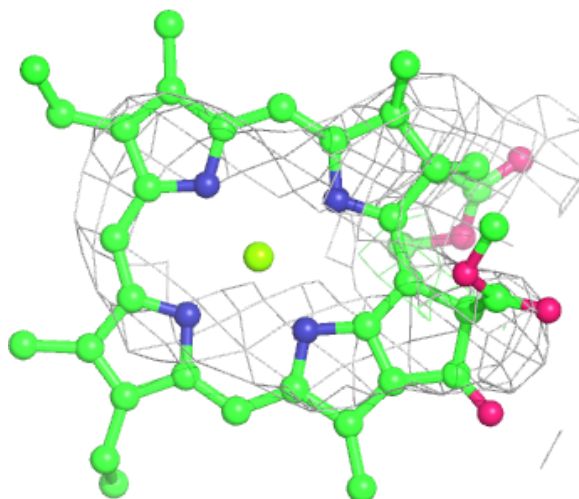
Electron density around CLA 3 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



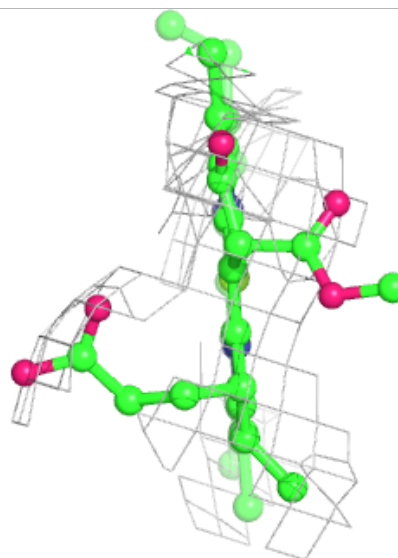
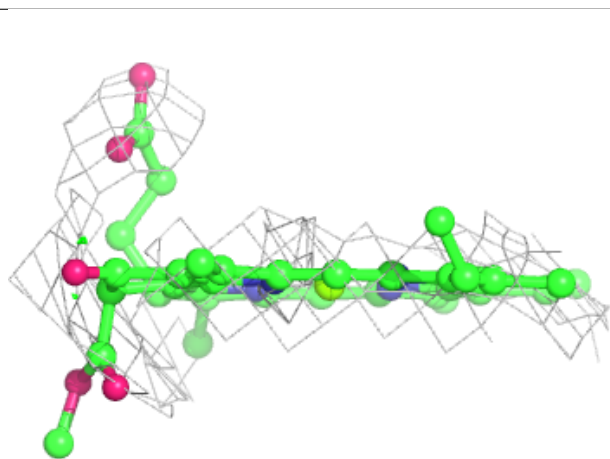
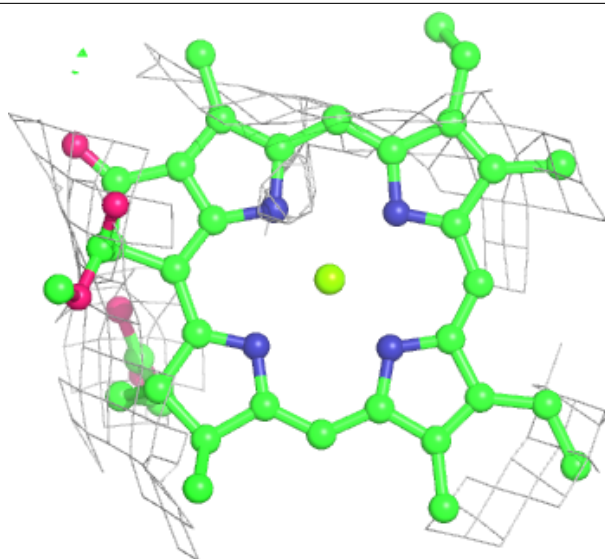
Electron density around CLA A 1114:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



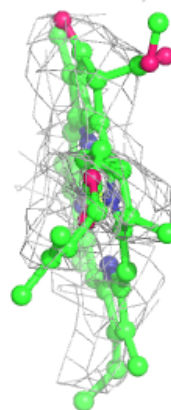
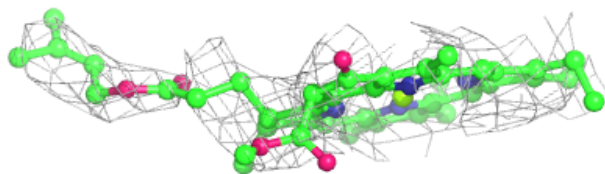
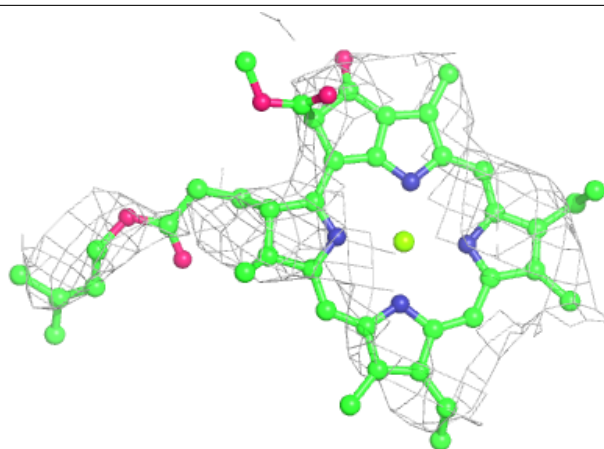
Electron density around CLA 3 606:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



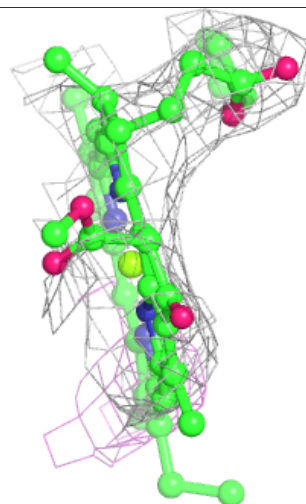
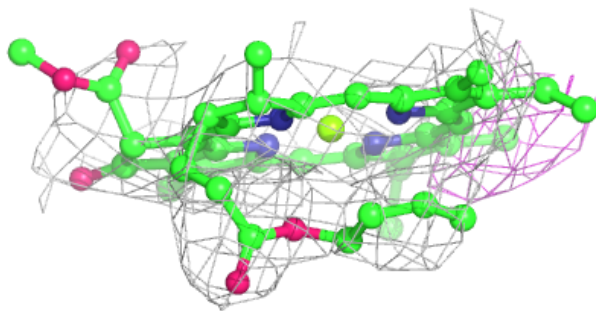
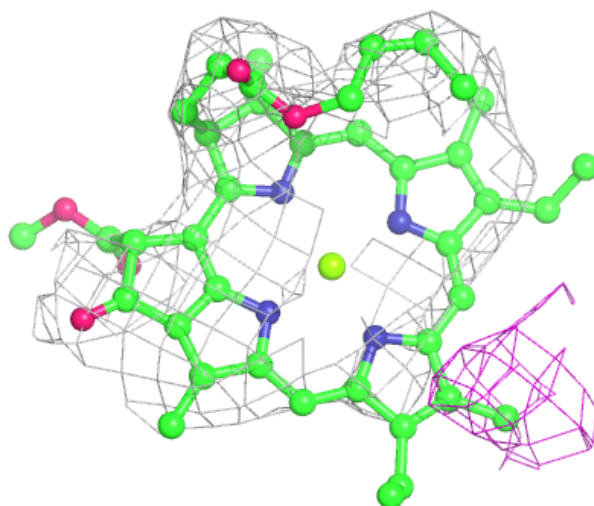
Electron density around CLA B 1022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



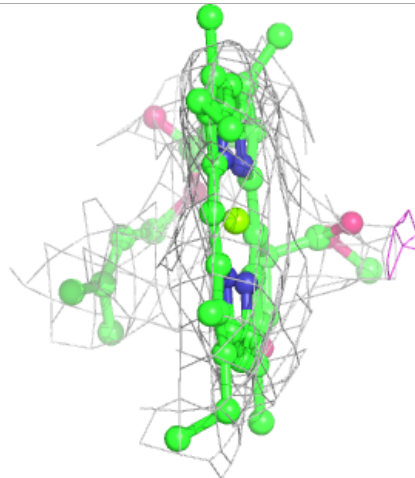
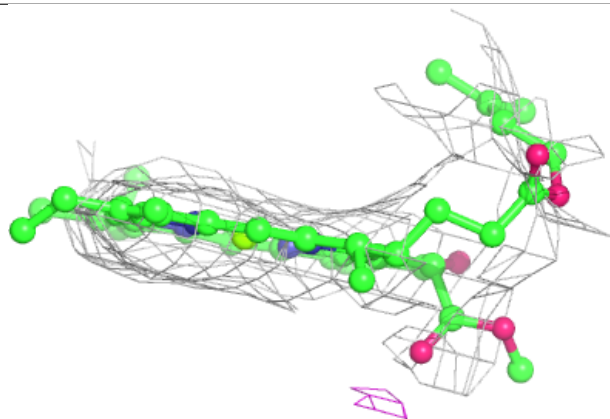
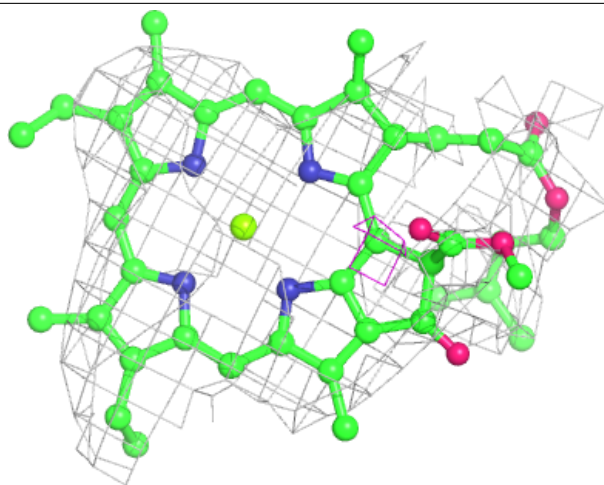
Electron density around CLA B 1215:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



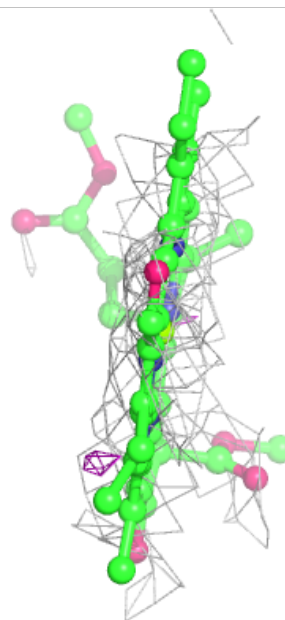
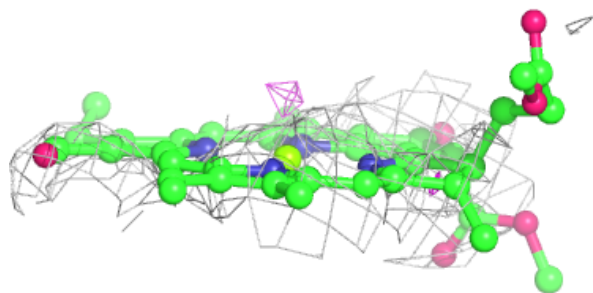
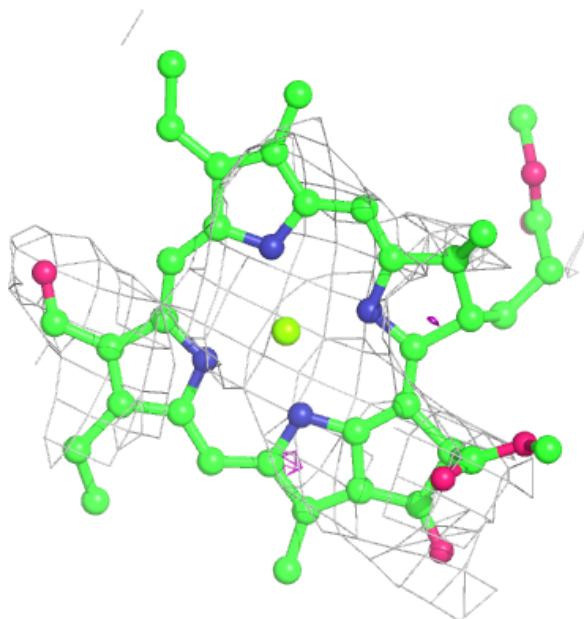
Electron density around CLA B 1238:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



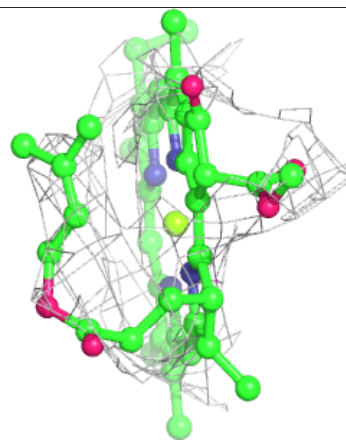
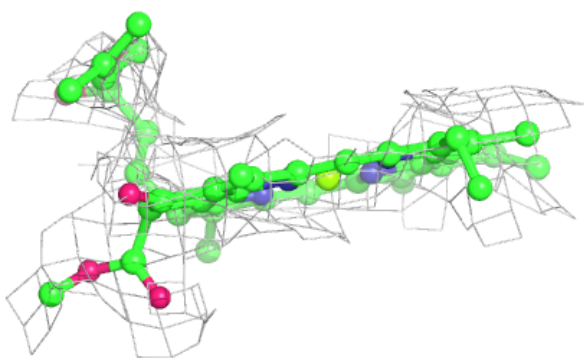
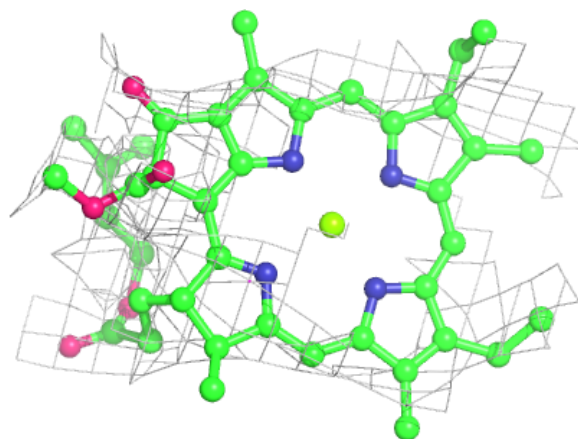
Electron density around CHL 3 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



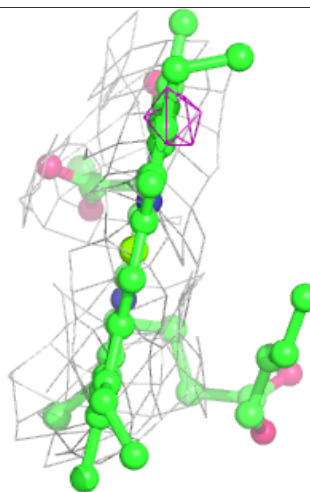
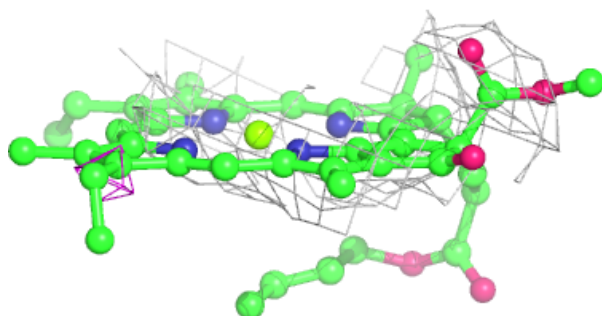
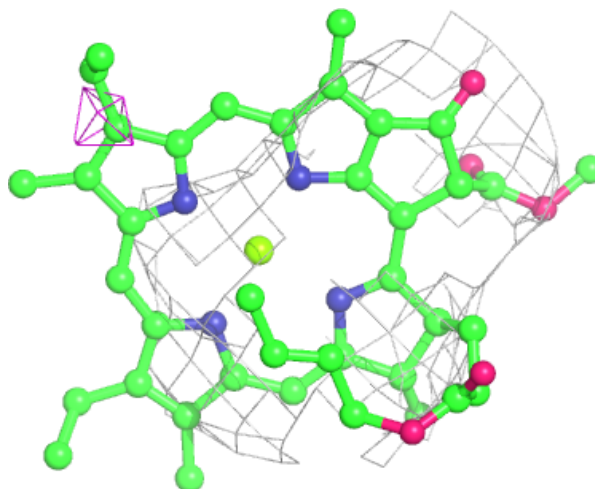
Electron density around CLA A 1141:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



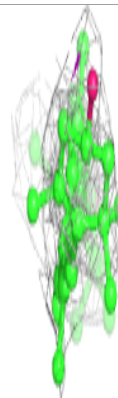
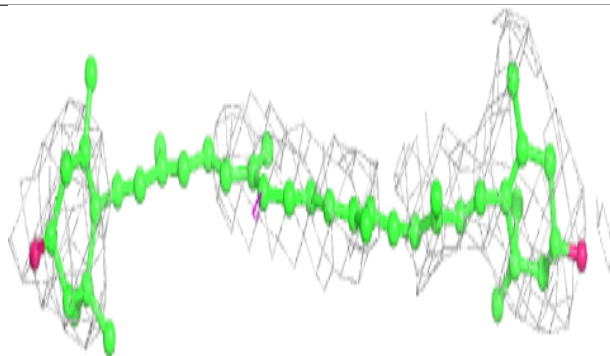
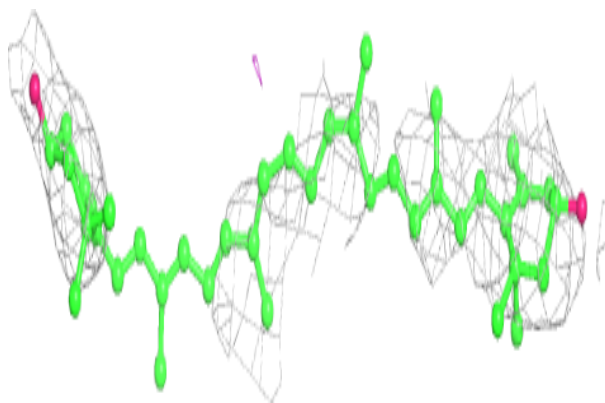
Electron density around CLA A 1116:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

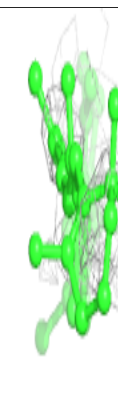
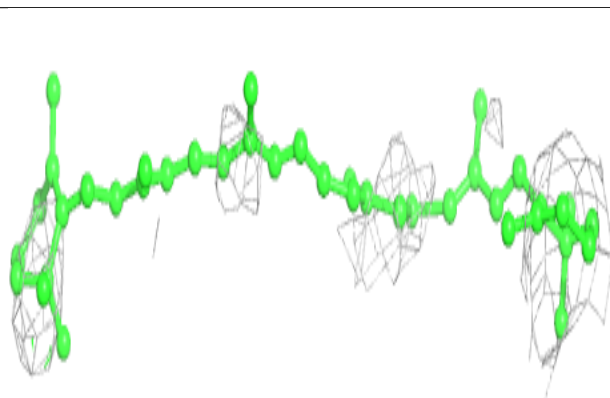
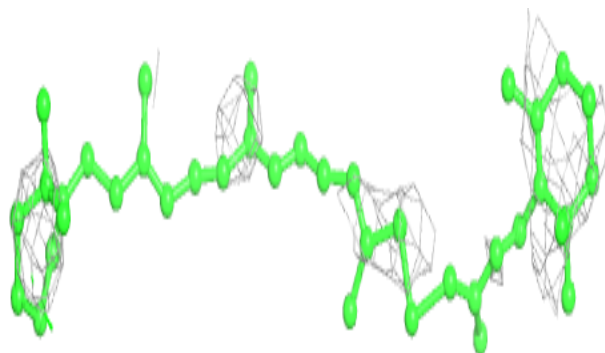


Electron density around LUT 1 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

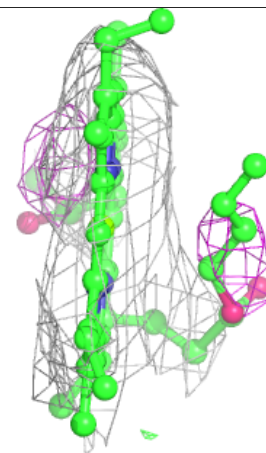
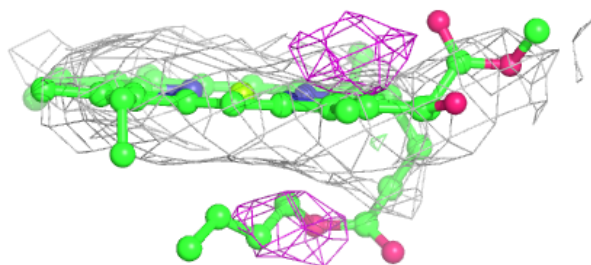
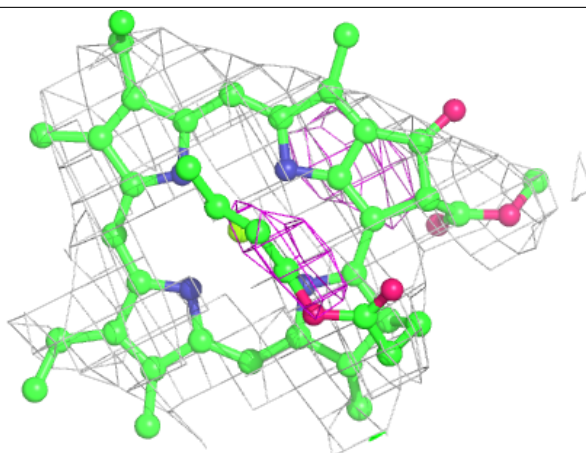
**Electron density around BCR A 4005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

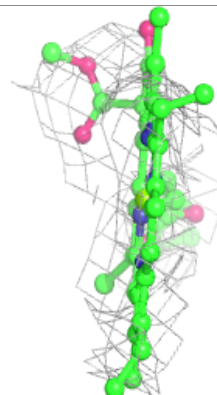
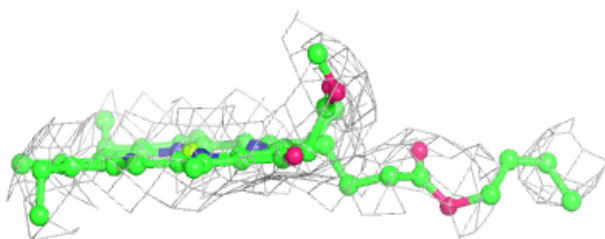
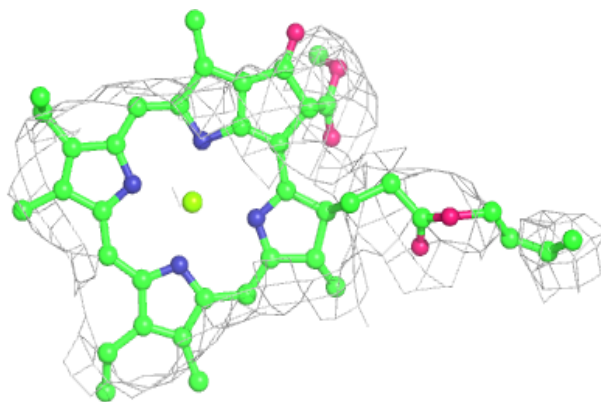


Electron density around CLA B 1211:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

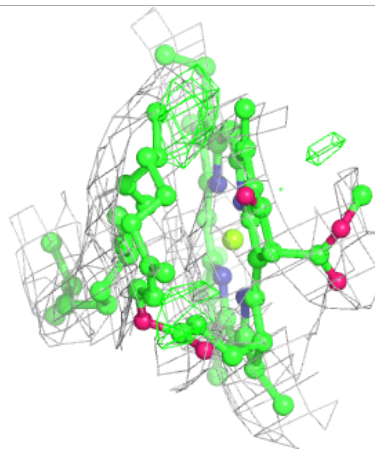
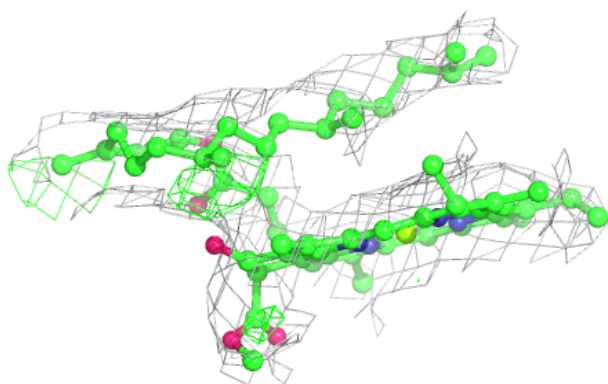
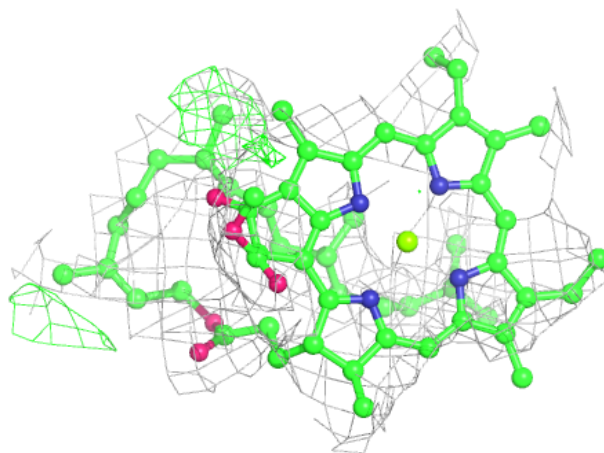
**Electron density around CLA A 1135:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



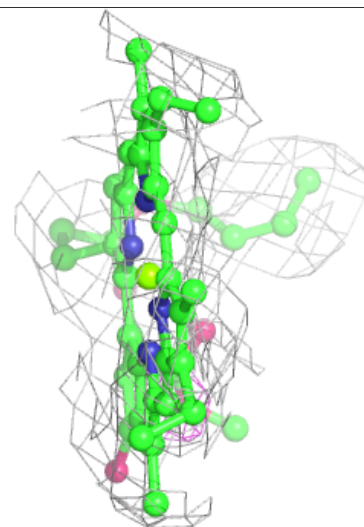
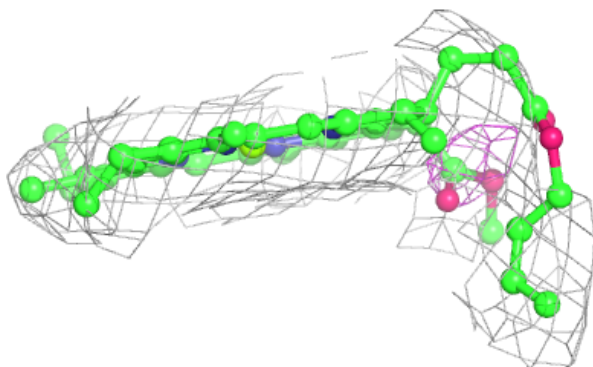
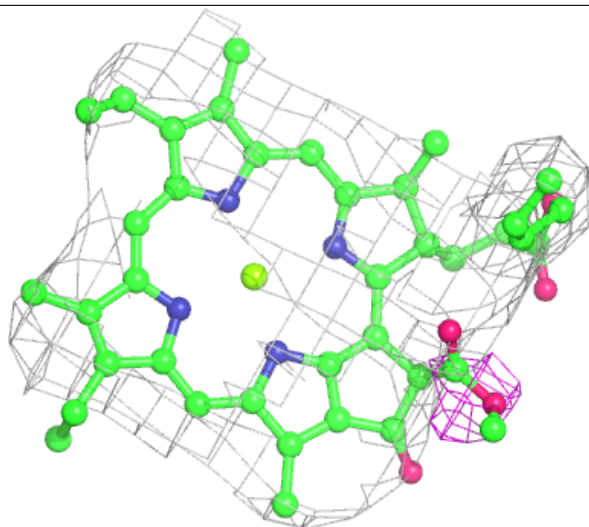
Electron density around CLA 2 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



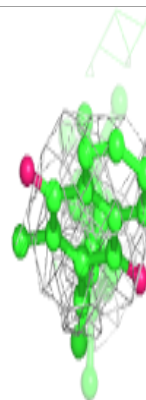
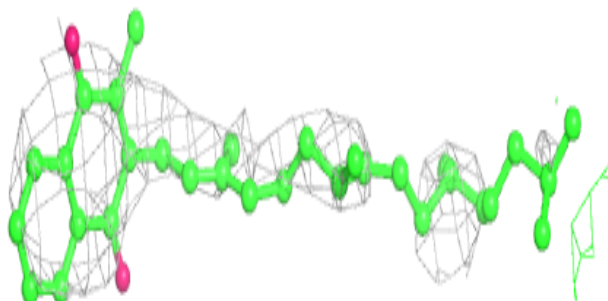
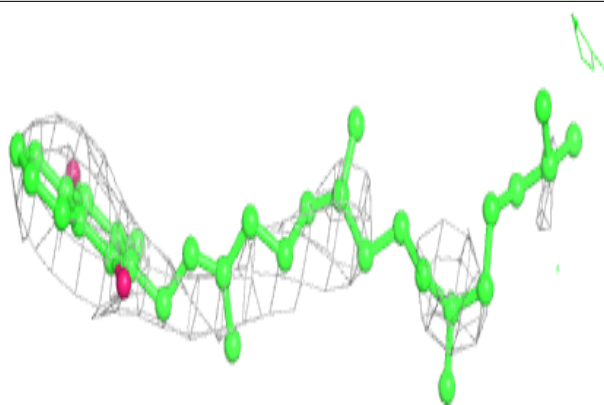
Electron density around CLA 2 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



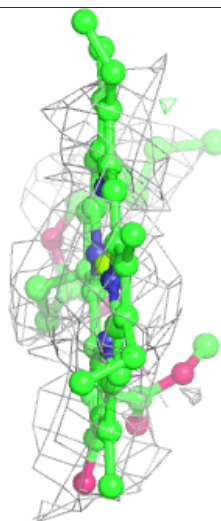
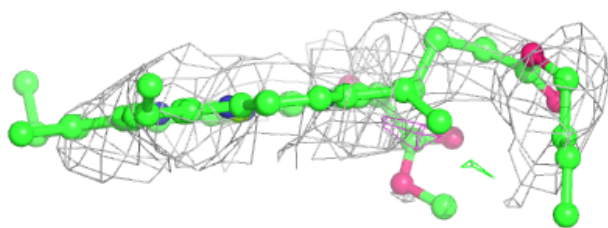
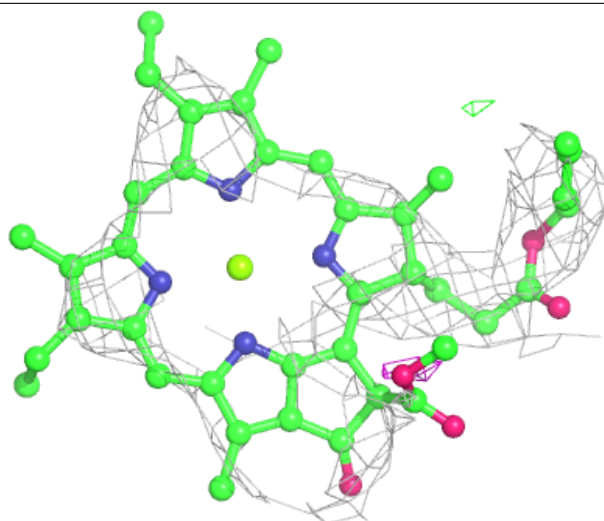
Electron density around PQN A 2001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



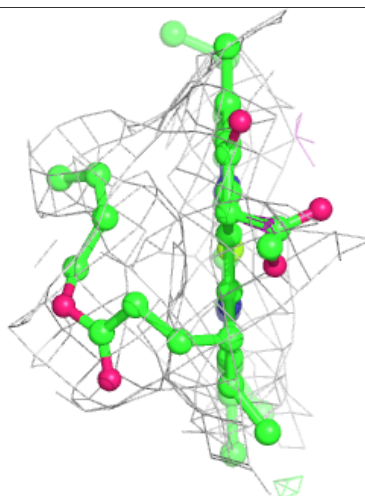
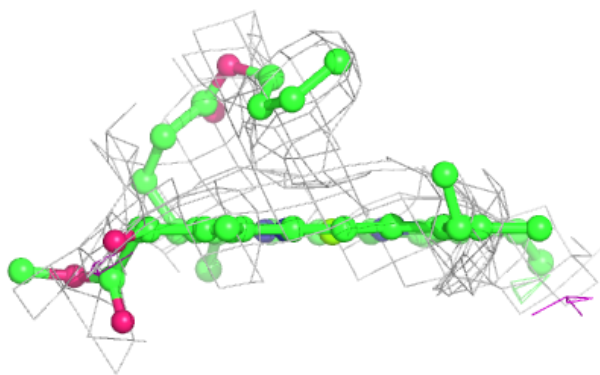
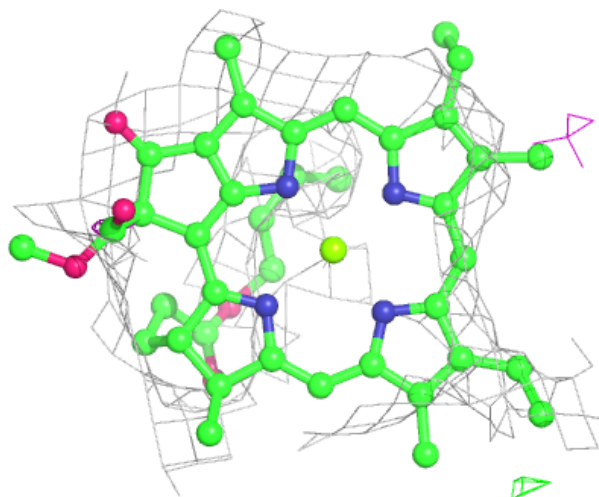
Electron density around CLA B 1221:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



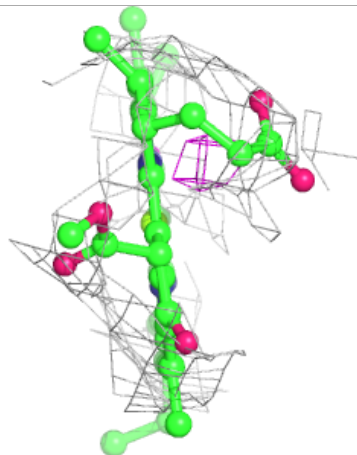
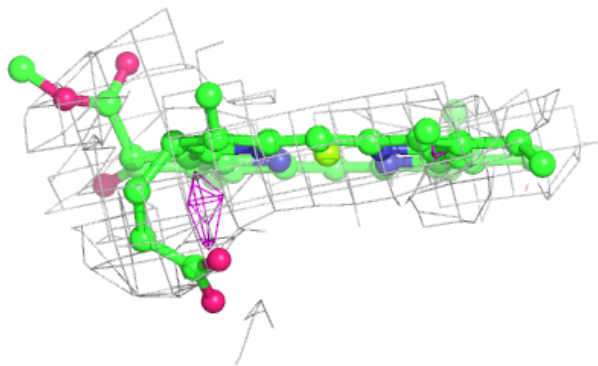
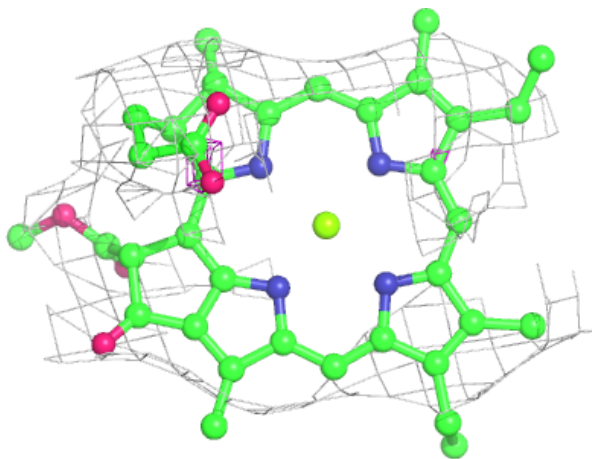
Electron density around CLA B 1218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



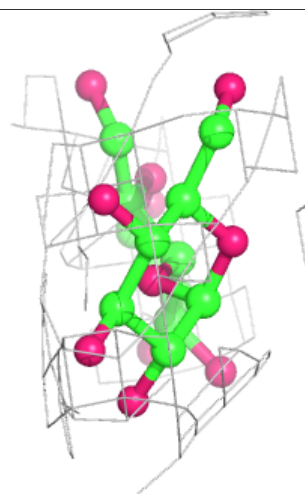
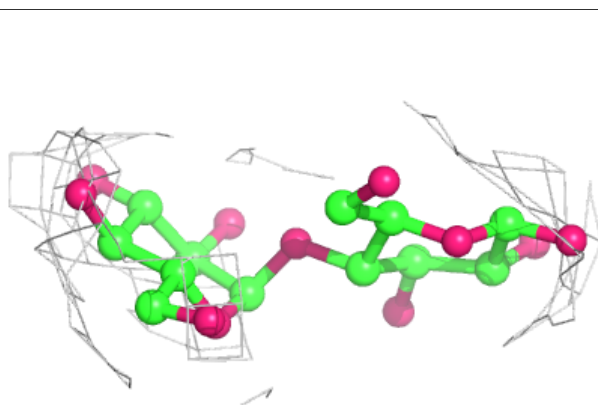
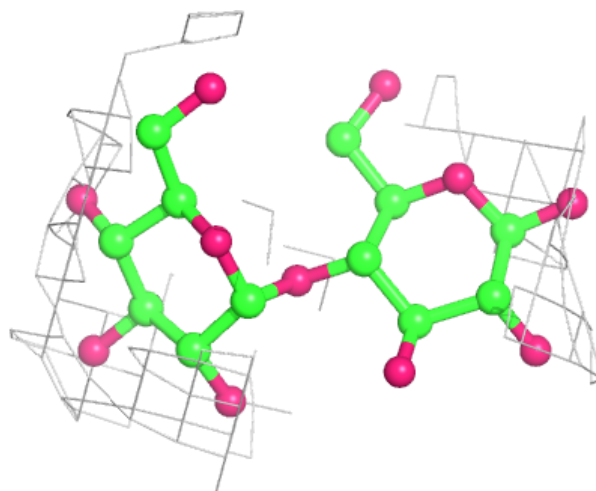
Electron density around CLA 1 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



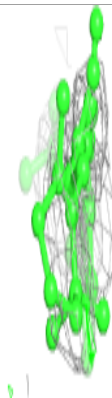
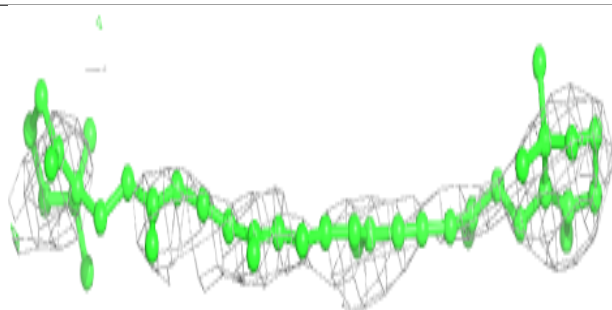
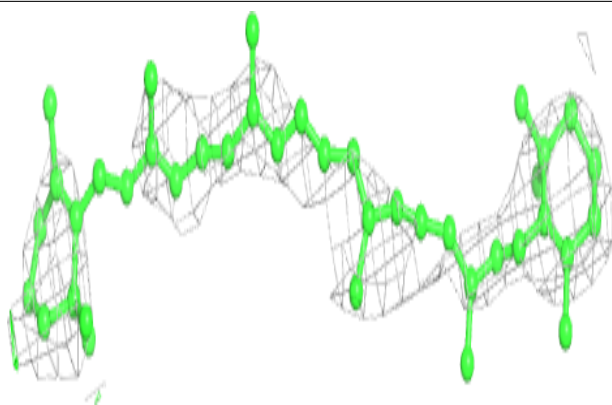
Electron density around LMT 2 821:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

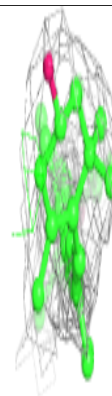
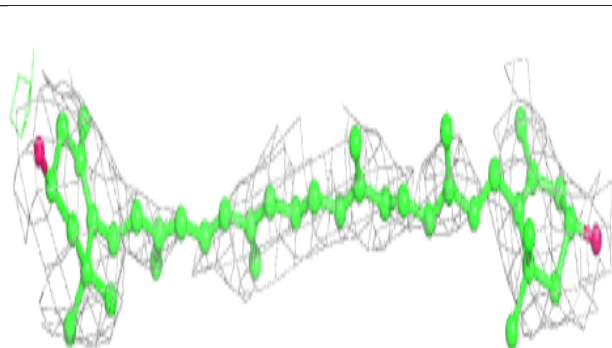
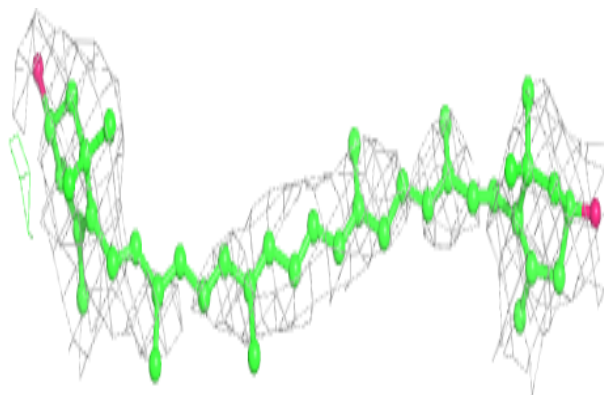


Electron density around BCR J 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

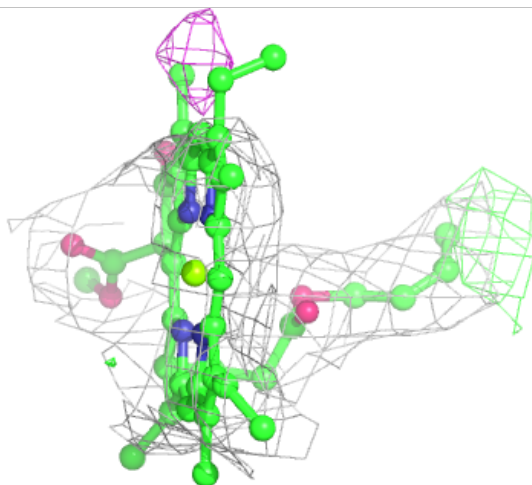
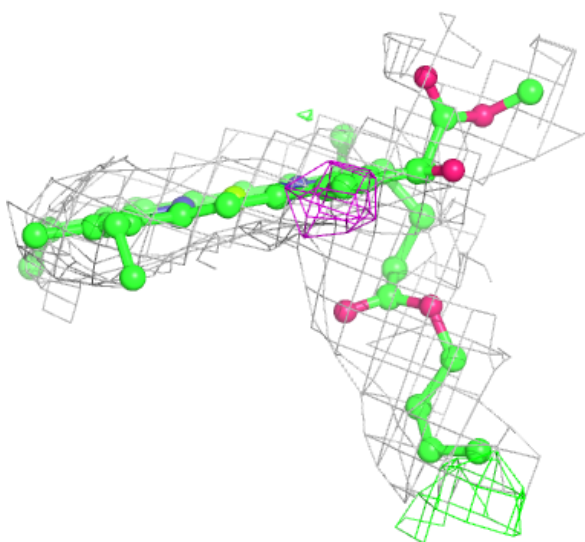
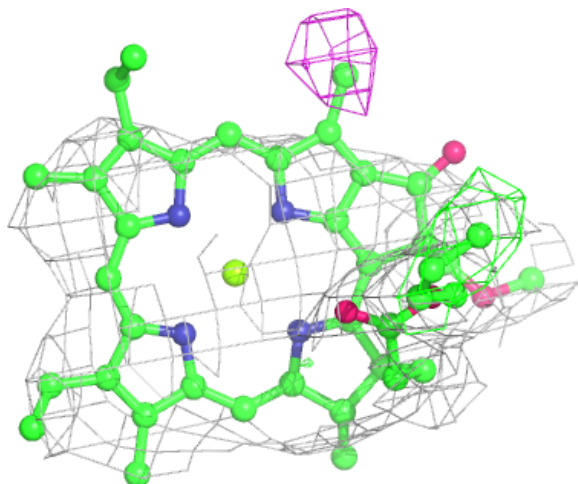
**Electron density around LUT 4 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



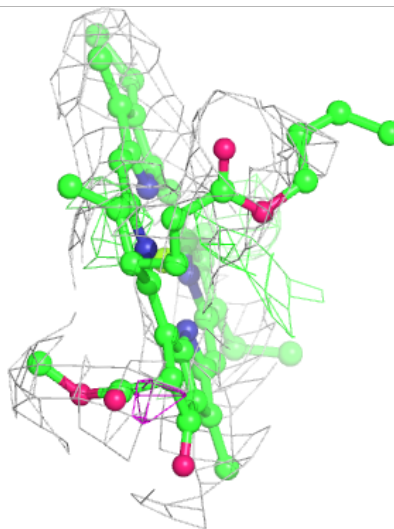
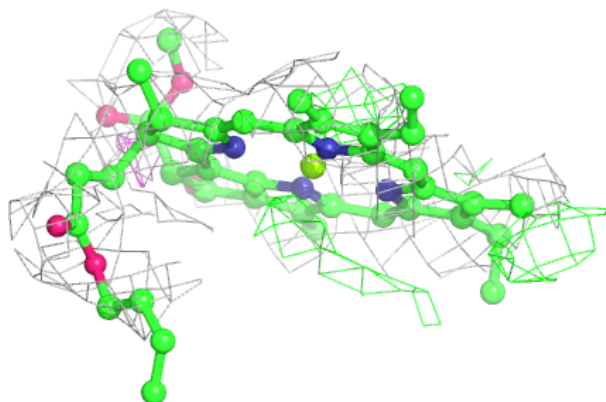
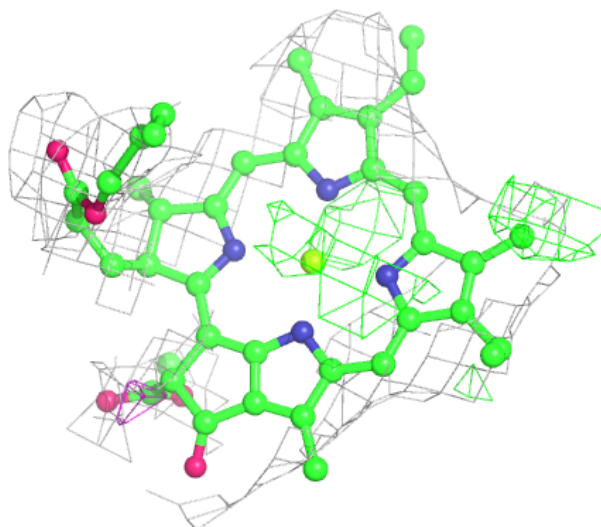
Electron density around CLA A 1126:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



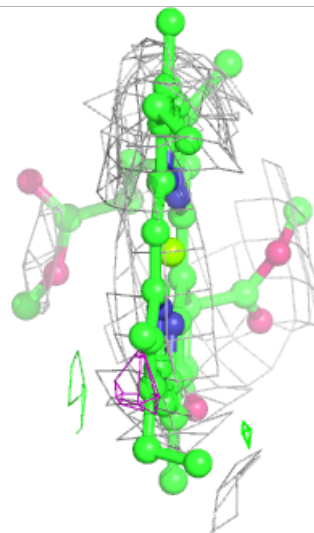
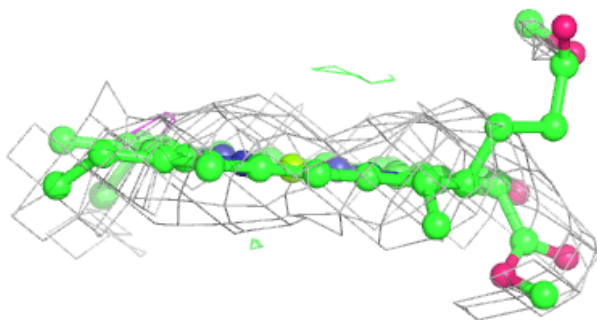
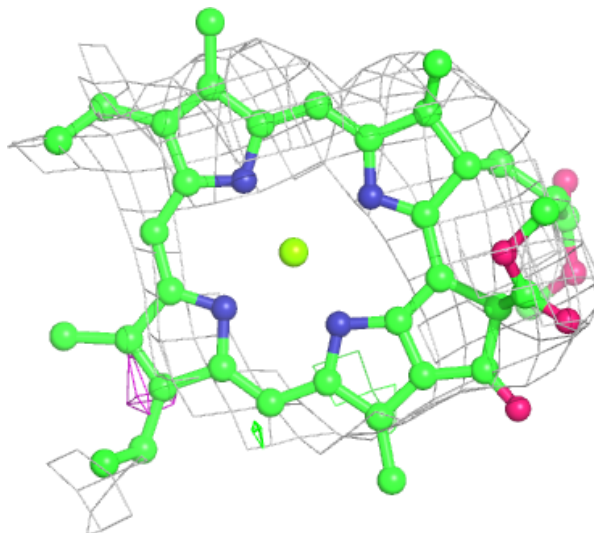
Electron density around CLA 4 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



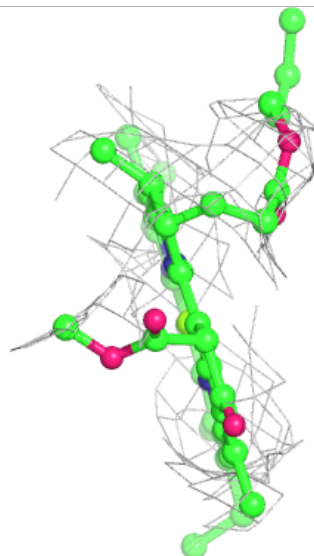
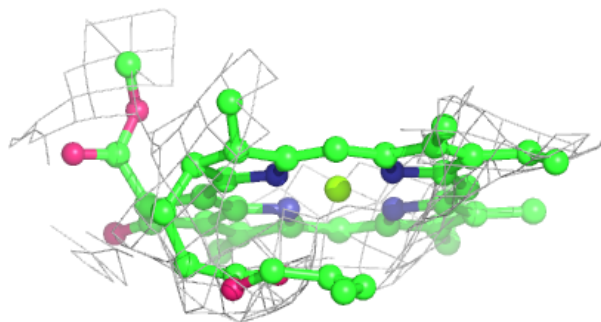
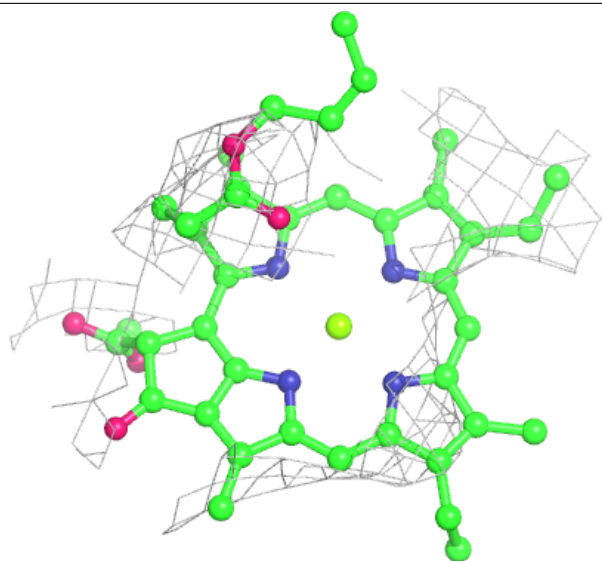
Electron density around CLA A 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



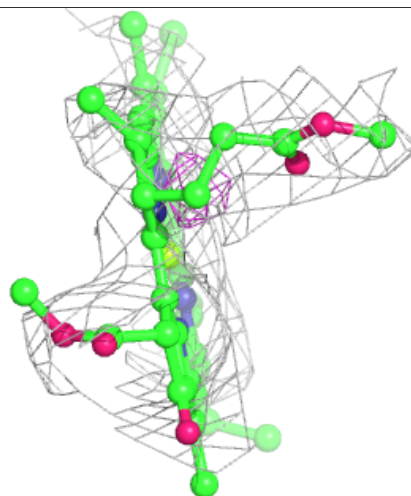
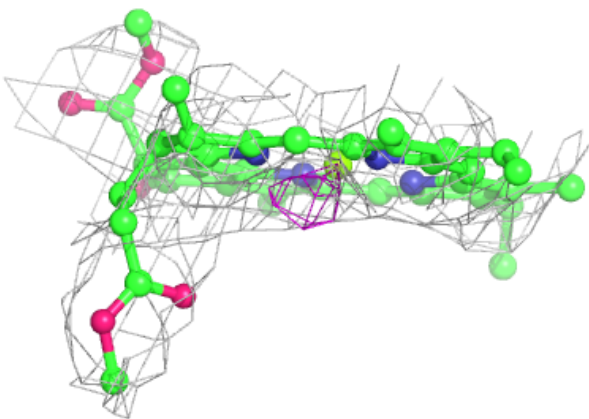
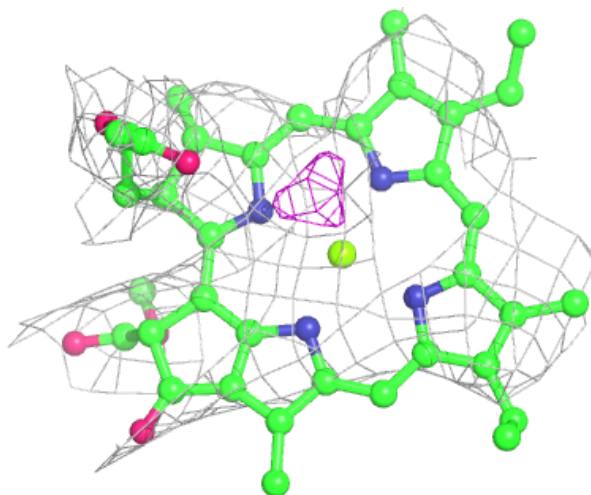
Electron density around CLA A 1134:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



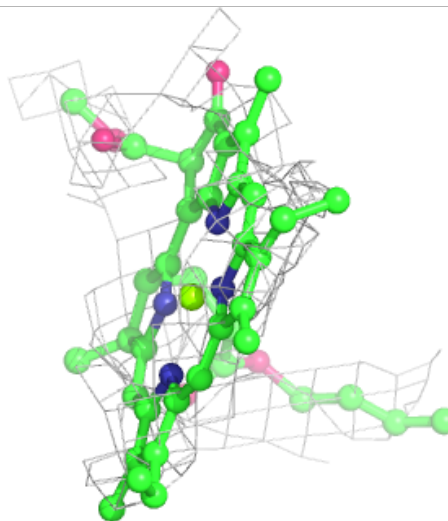
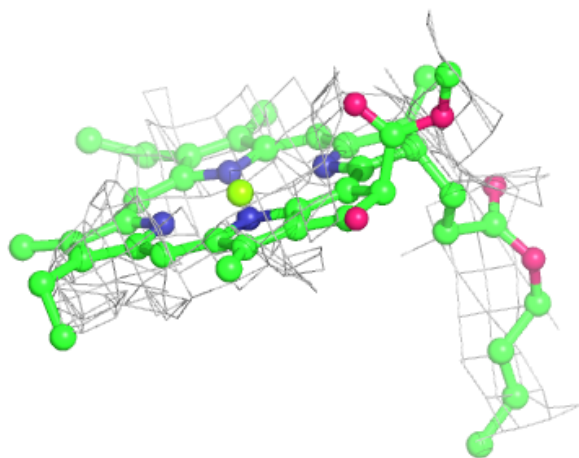
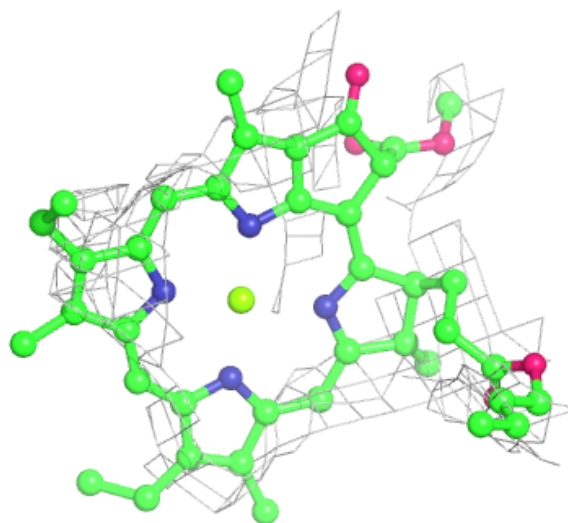
Electron density around CLA 2 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



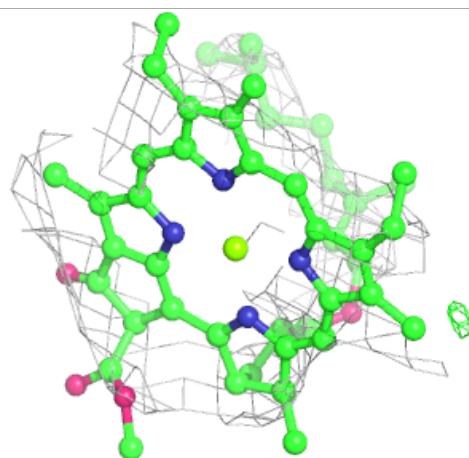
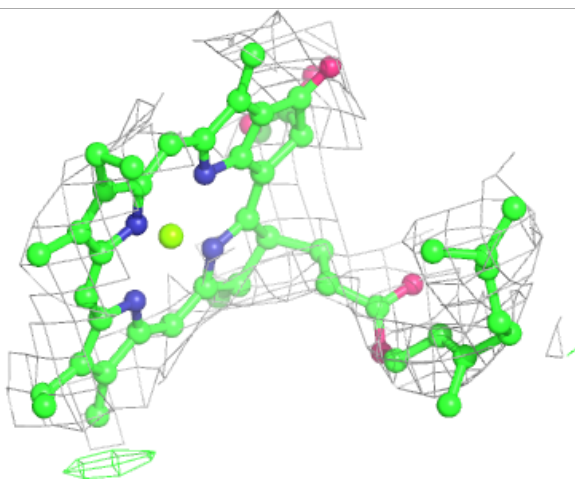
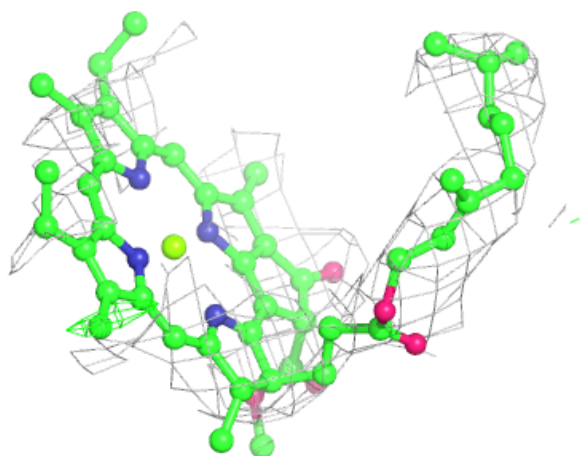
Electron density around CLA 3 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



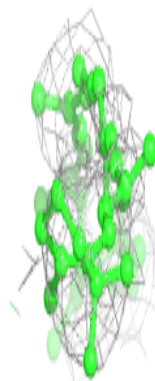
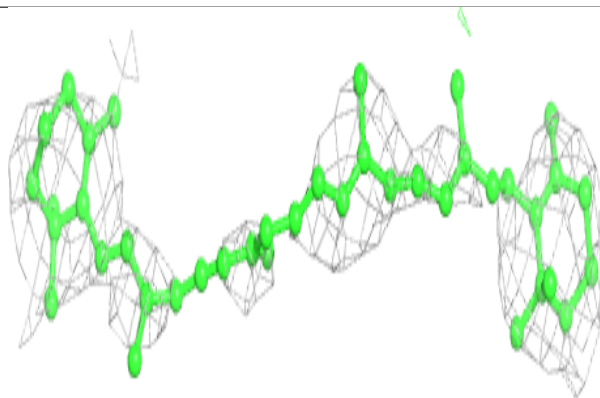
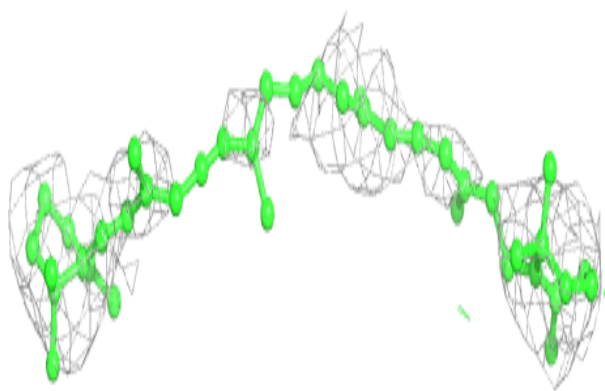
Electron density around CLA 3 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



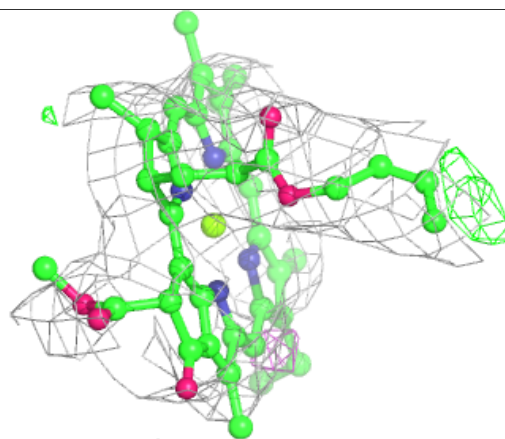
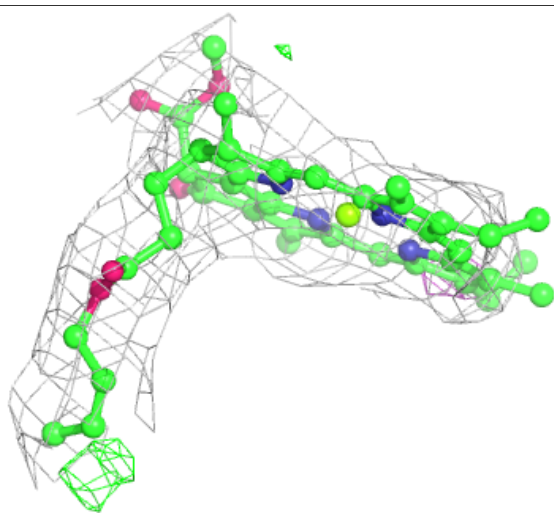
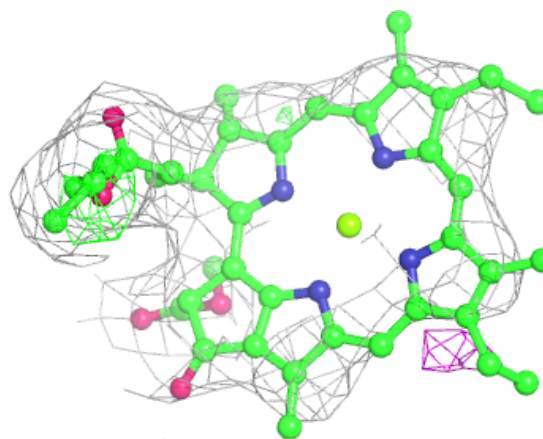
Electron density around BCR J 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



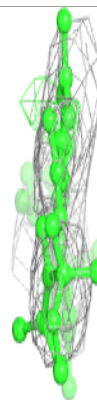
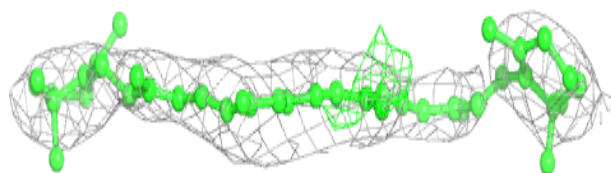
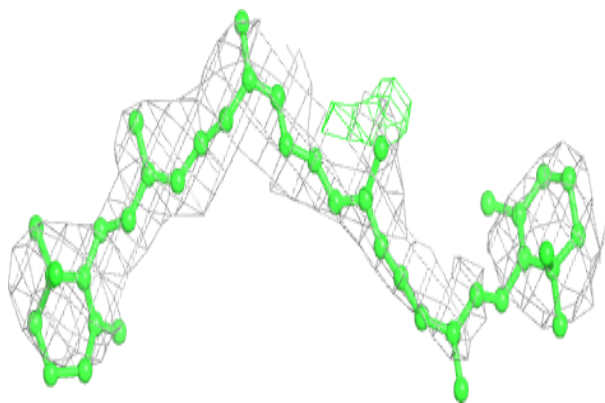
Electron density around CLA B 1236:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



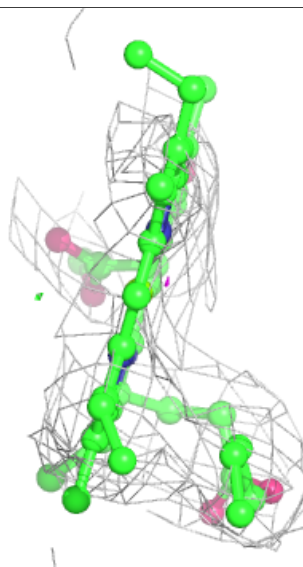
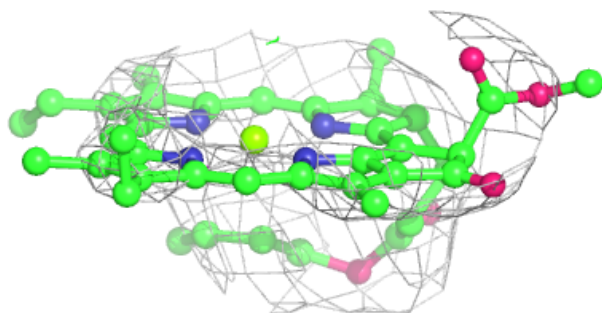
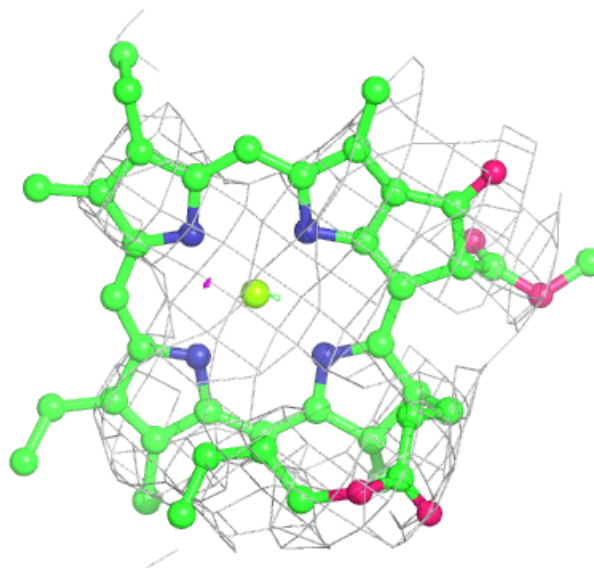
Electron density around BCR A 4006:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



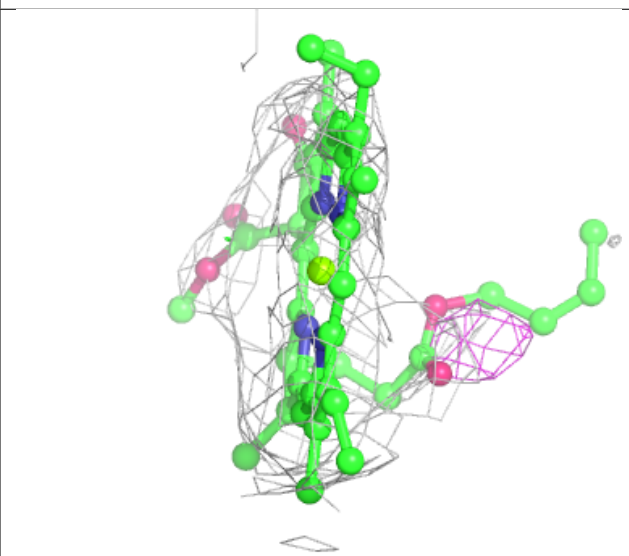
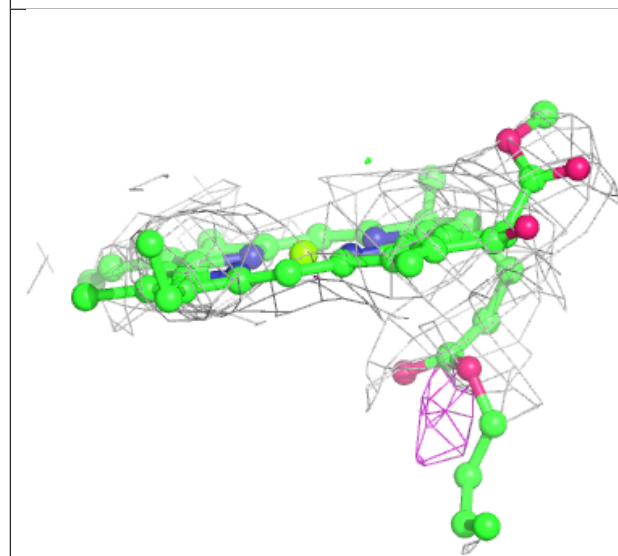
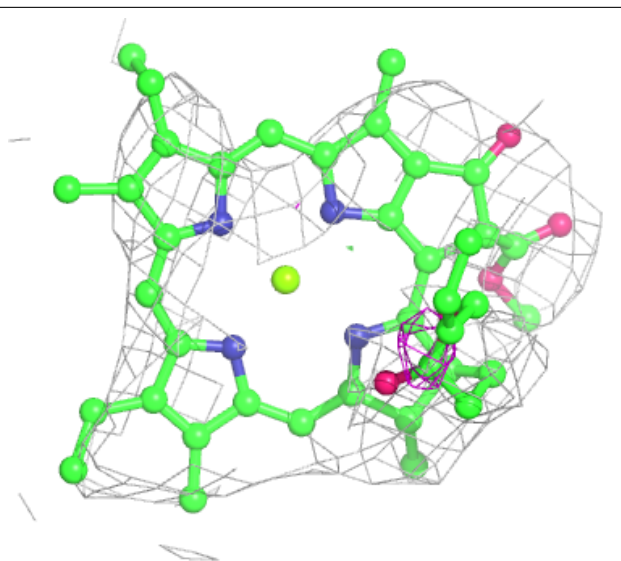
Electron density around CLA A 1117:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



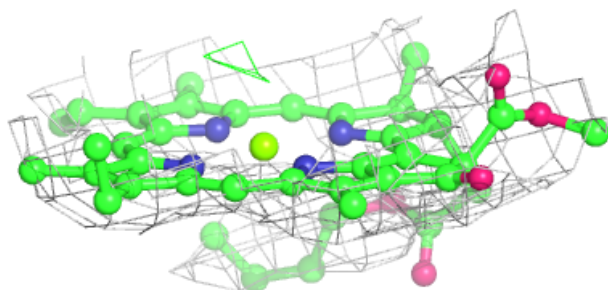
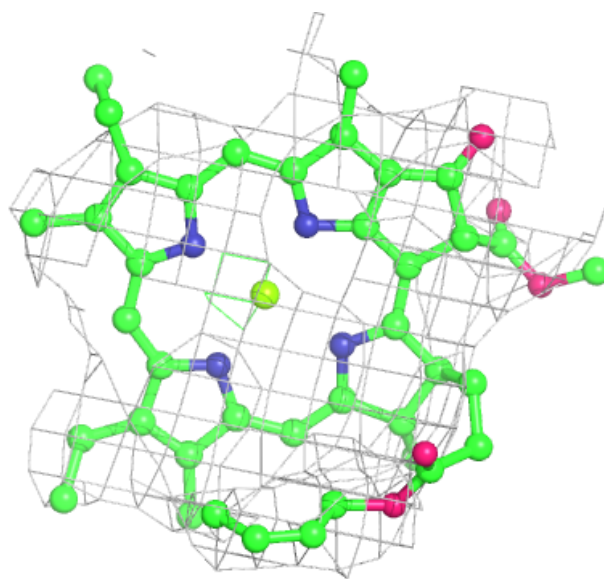
Electron density around CLA B 1226:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



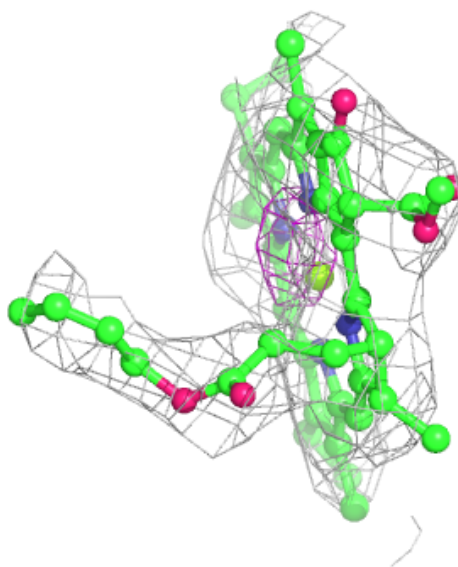
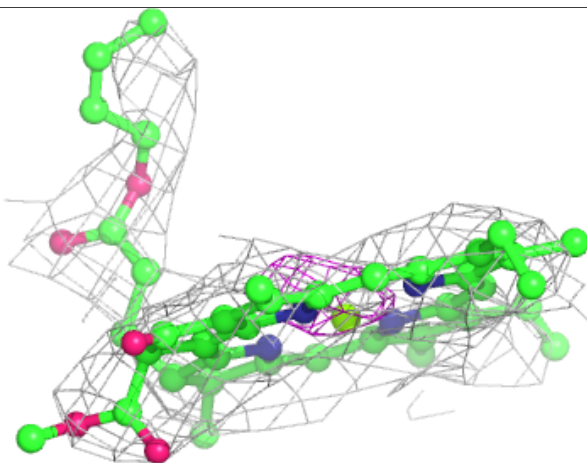
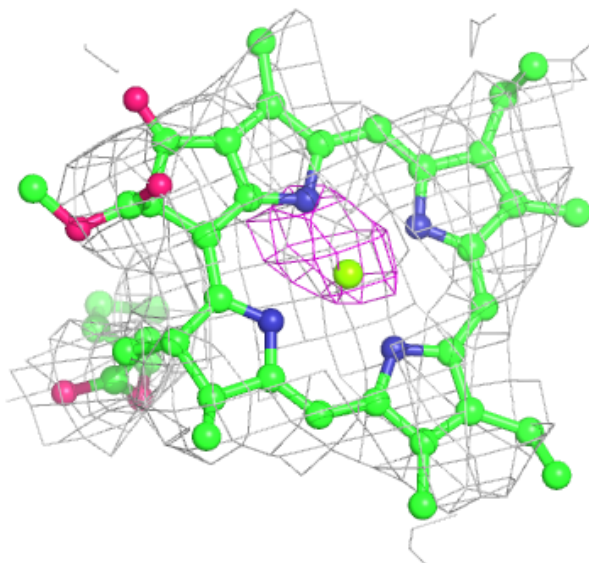
Electron density around CLA 1 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



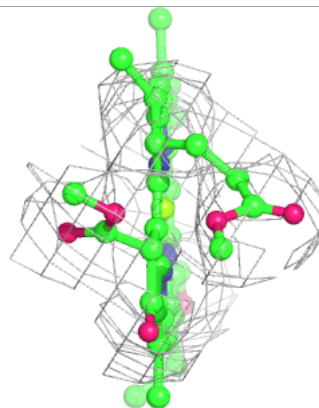
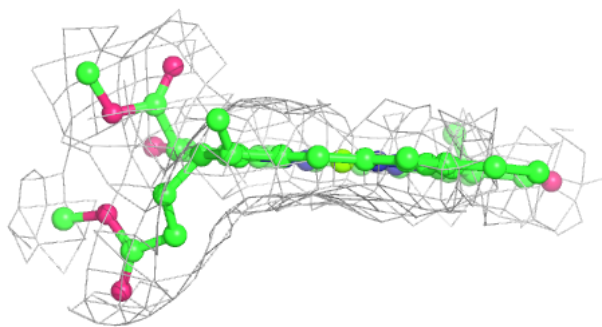
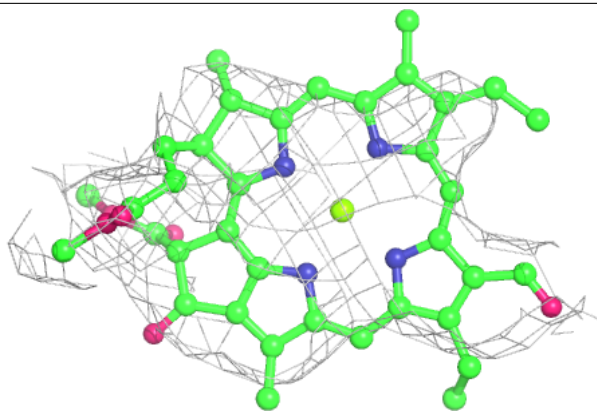
Electron density around CLA B 1219:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



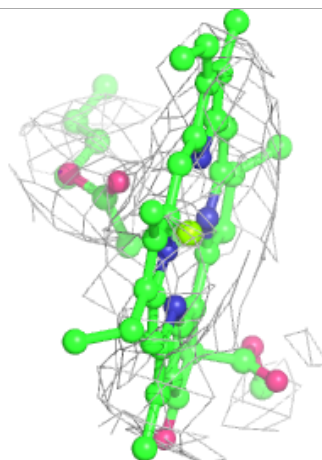
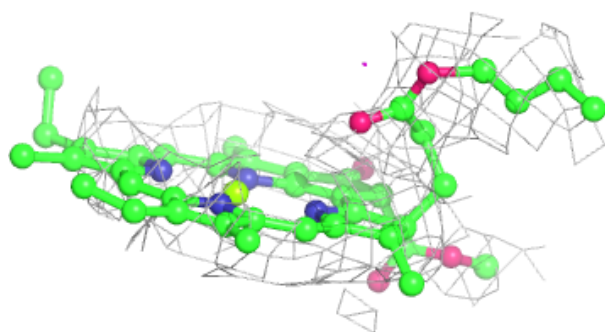
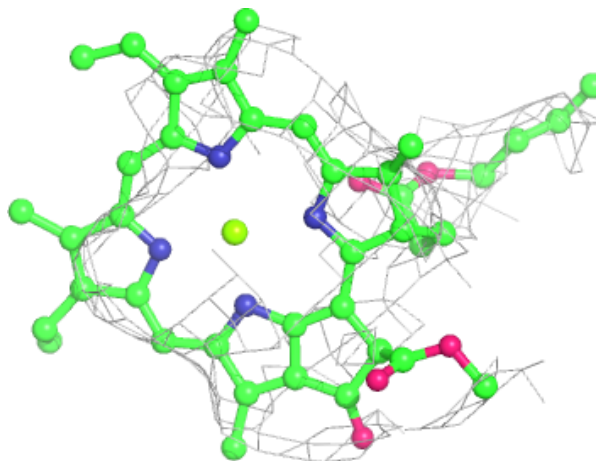
Electron density around CHL 1 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



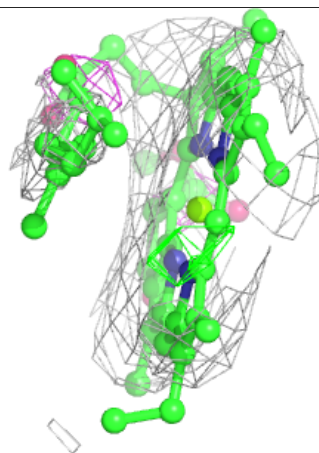
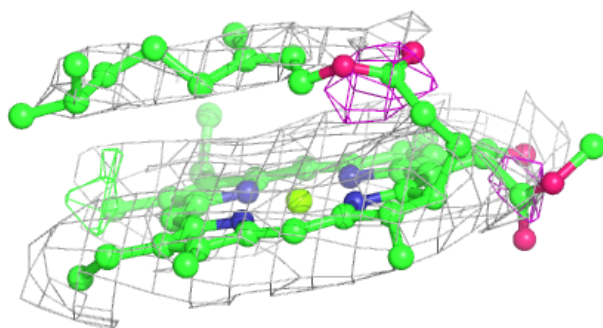
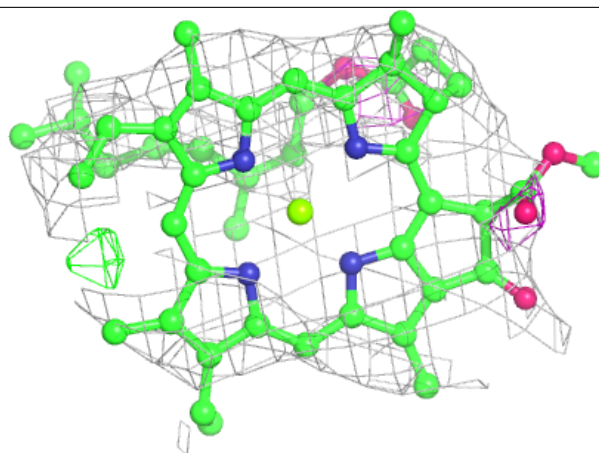
Electron density around CLA A 1124:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



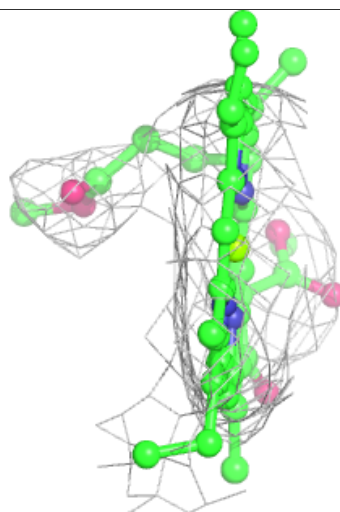
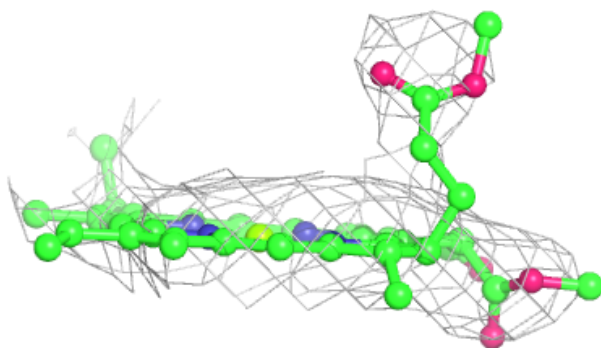
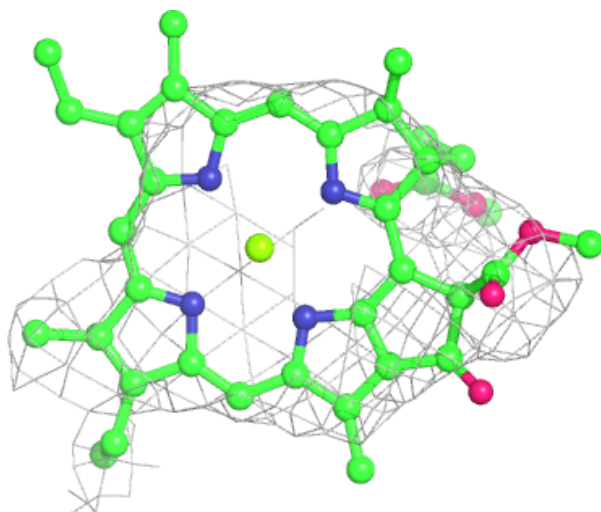
Electron density around CLA 4 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



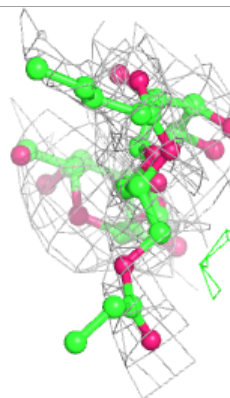
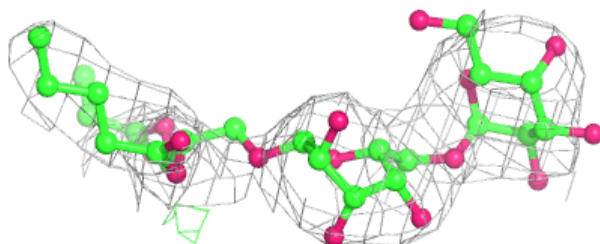
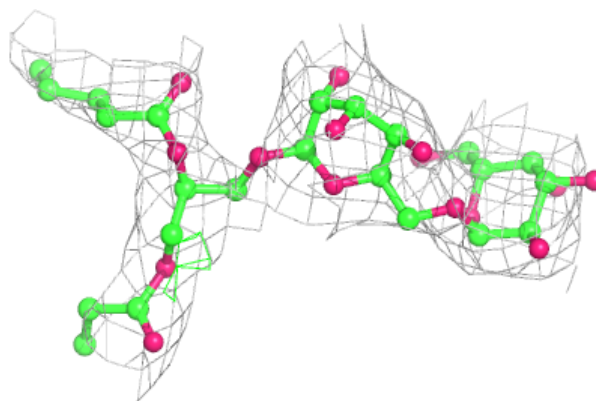
Electron density around CLA 3 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

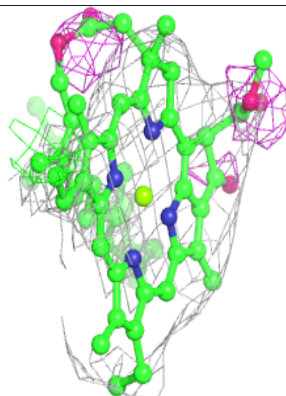
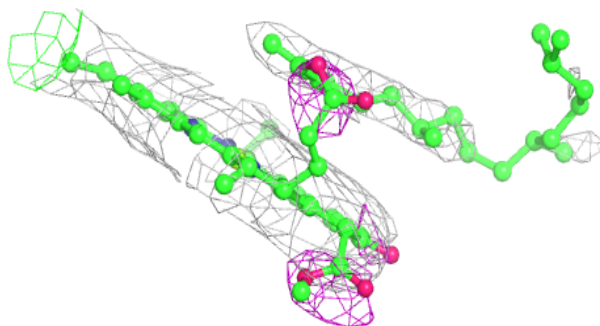
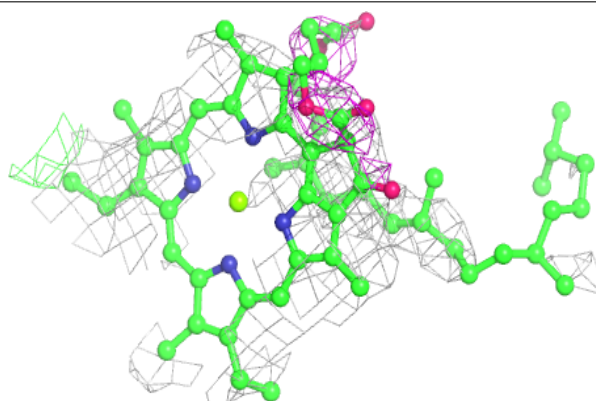


Electron density around DGD B 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

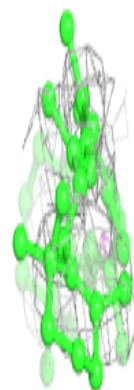
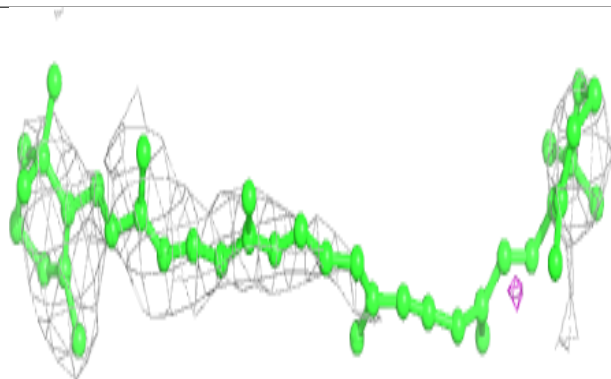
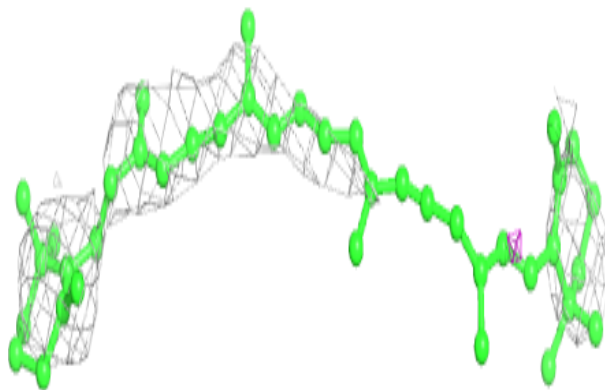
**Electron density around CLA 1 615:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



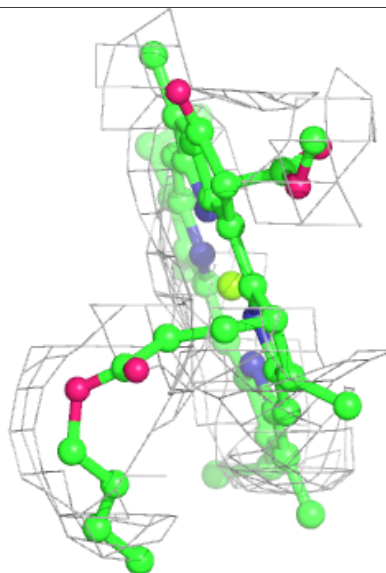
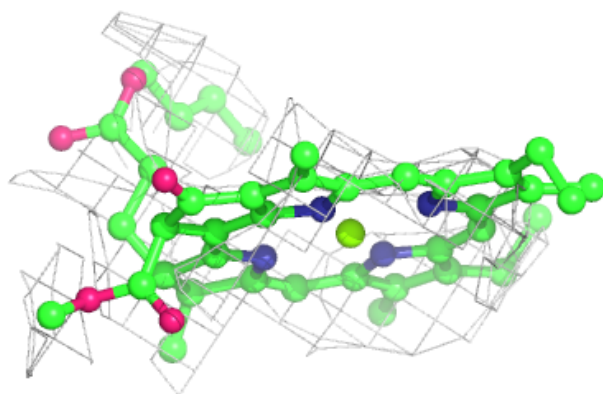
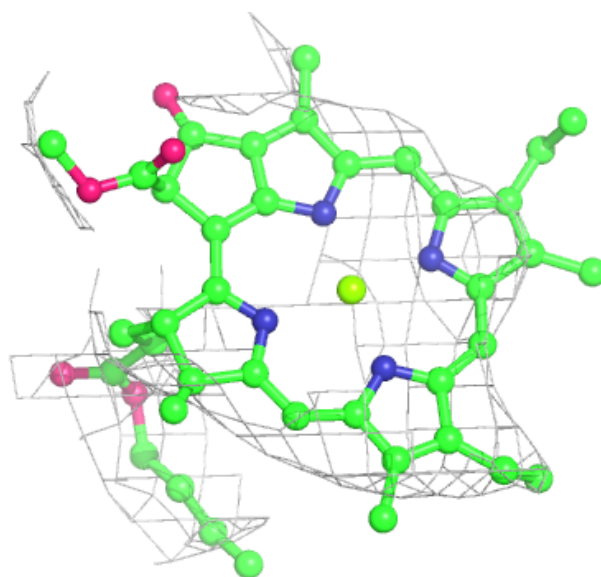
Electron density around BCR B 4006:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



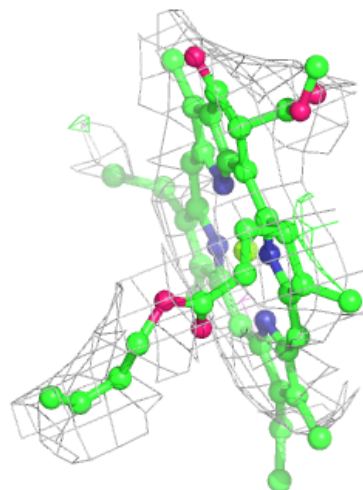
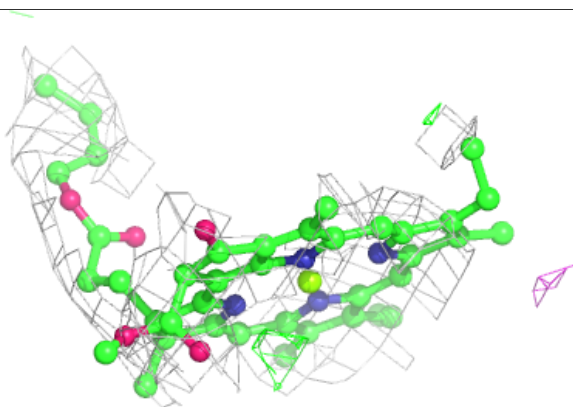
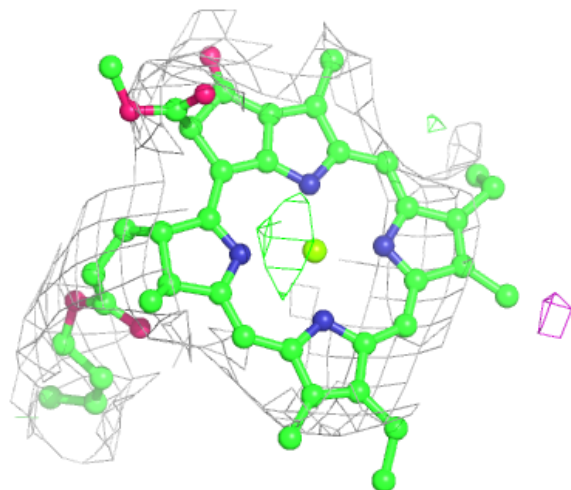
Electron density around CLA A 1120:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



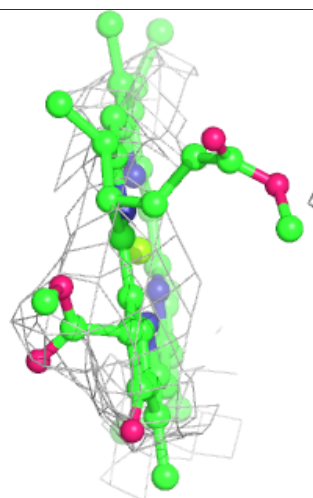
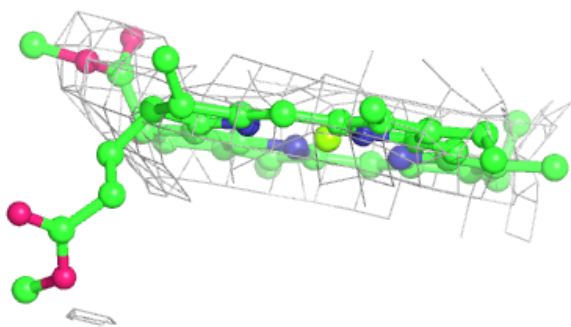
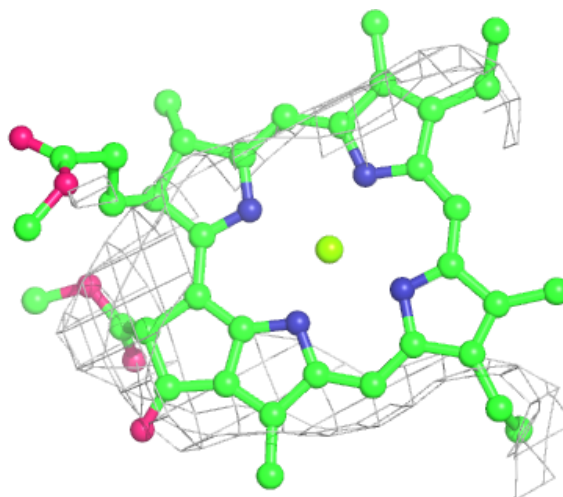
Electron density around CLA 2 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



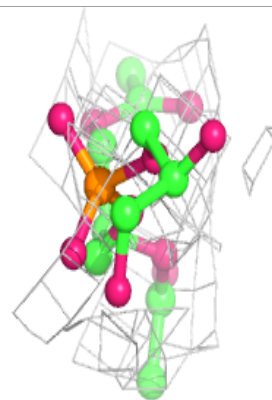
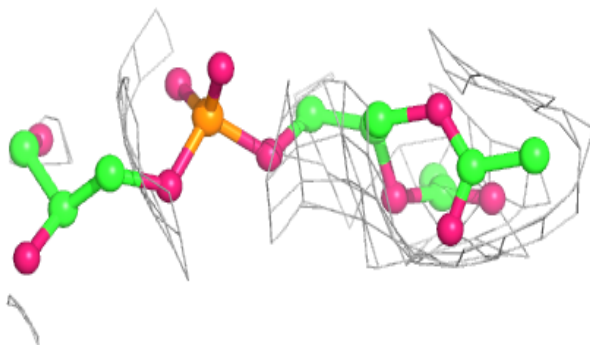
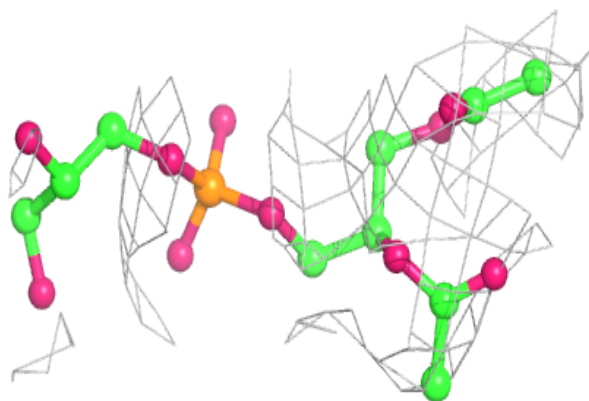
Electron density around CLA 3 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



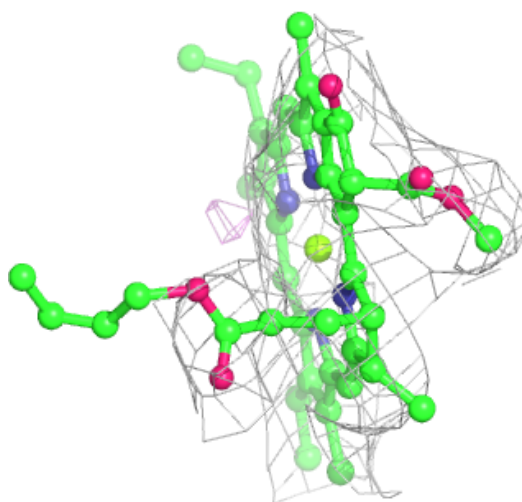
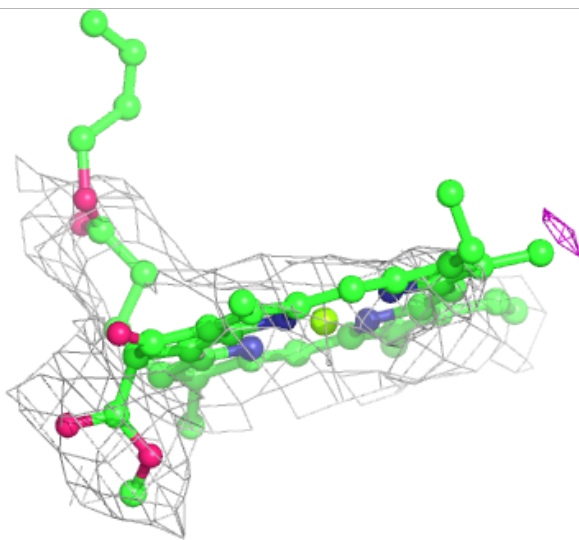
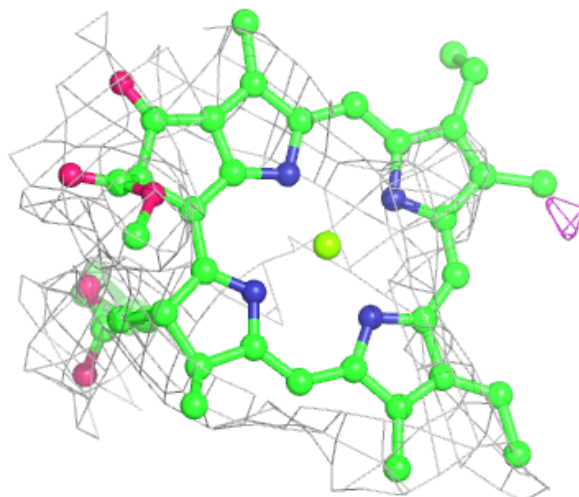
Electron density around LHG 2 801:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



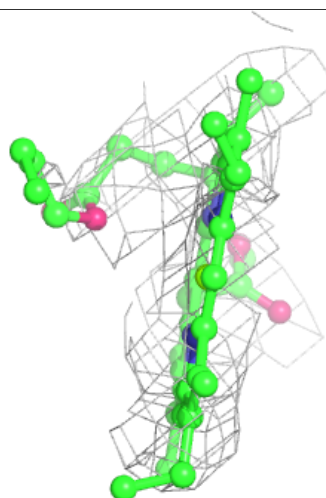
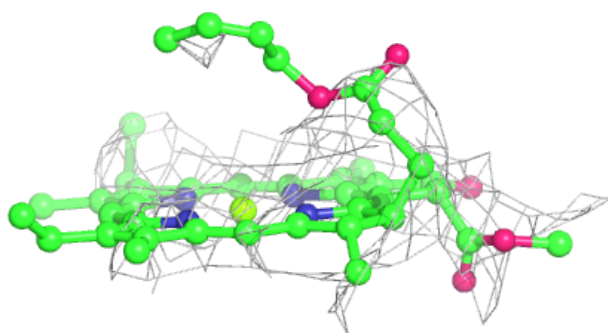
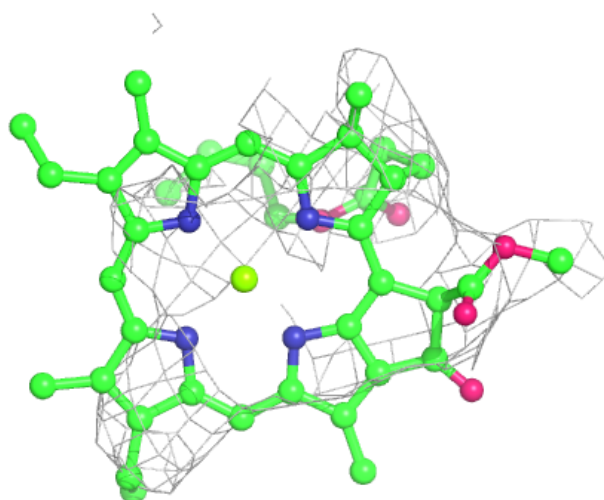
Electron density around CLA A 1128:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



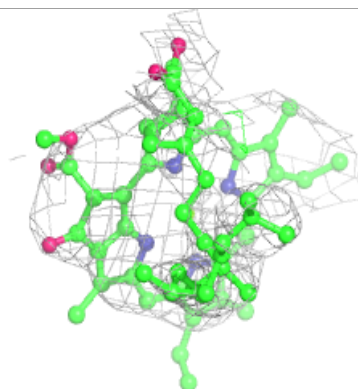
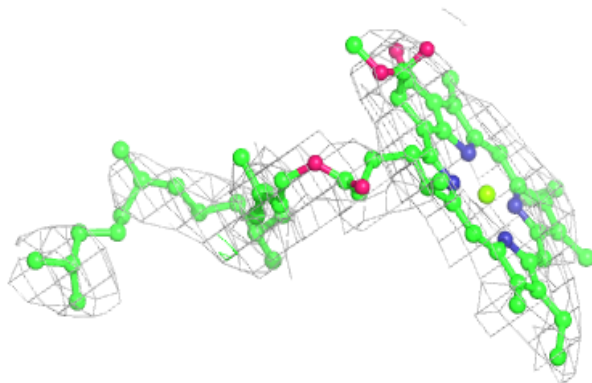
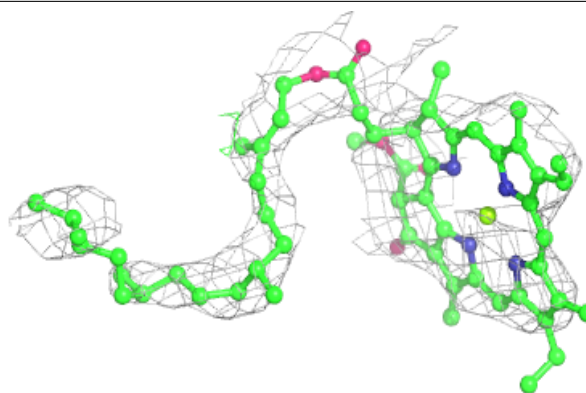
Electron density around CLA A 1119:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



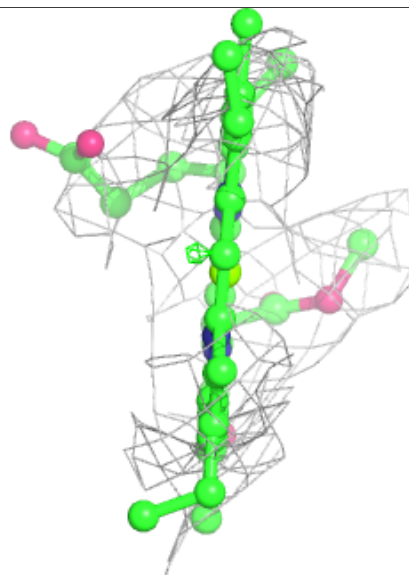
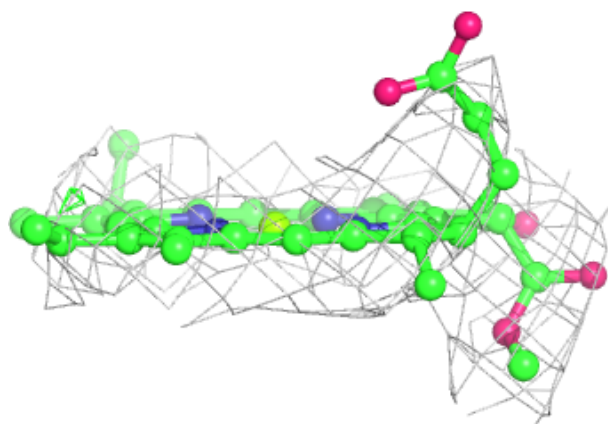
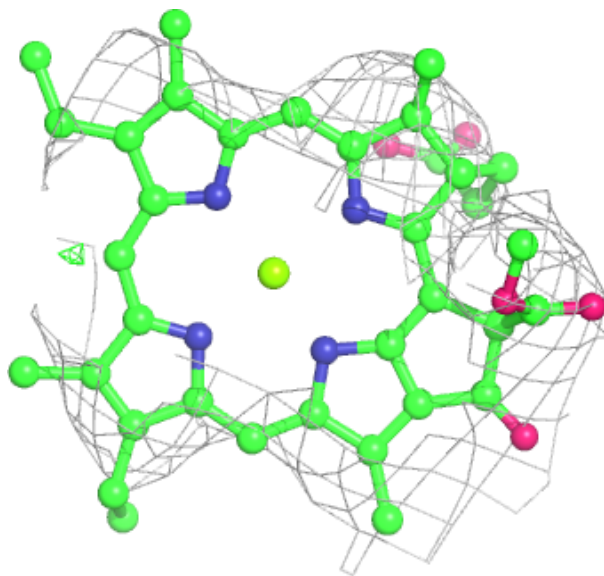
Electron density around CLA B 1021:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



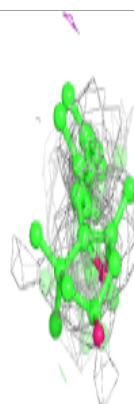
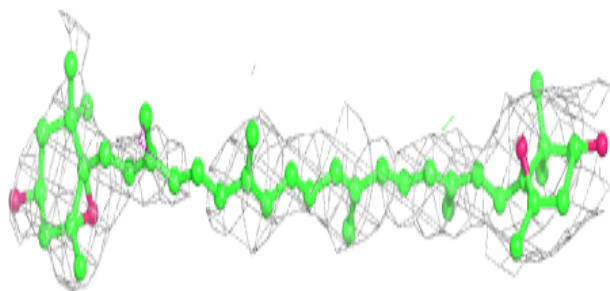
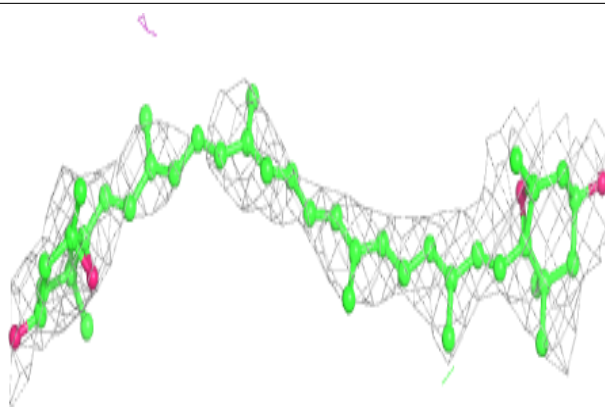
Electron density around CLA B 1212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



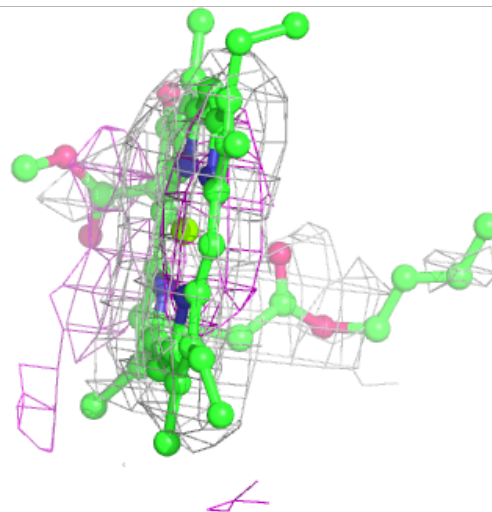
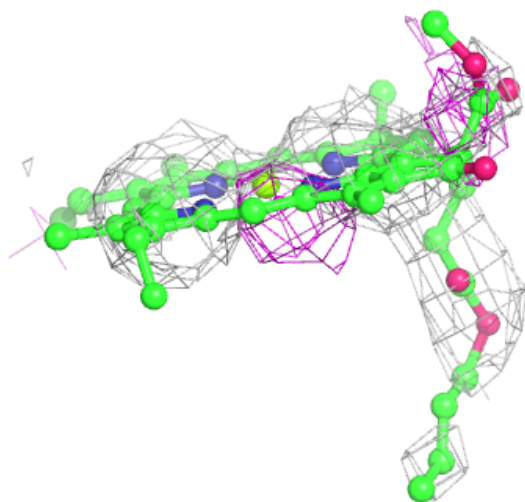
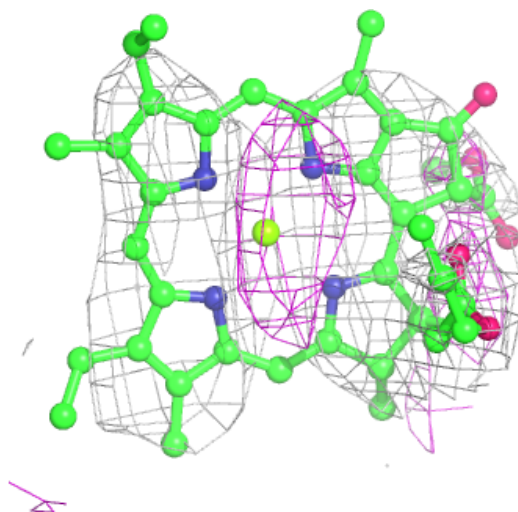
Electron density around XAT 4 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



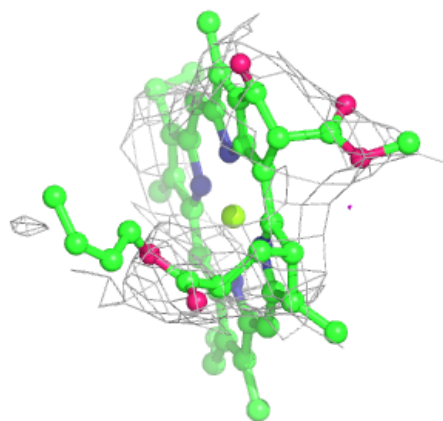
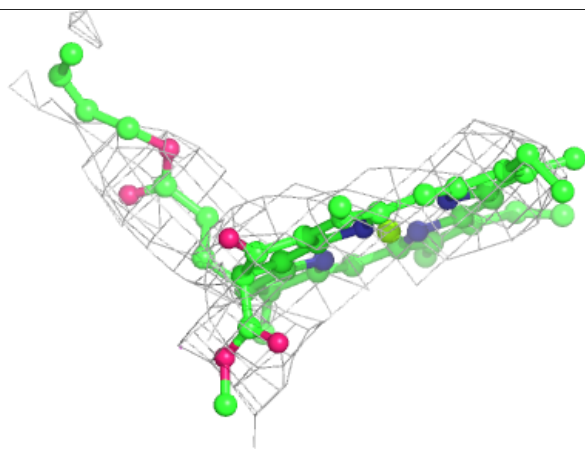
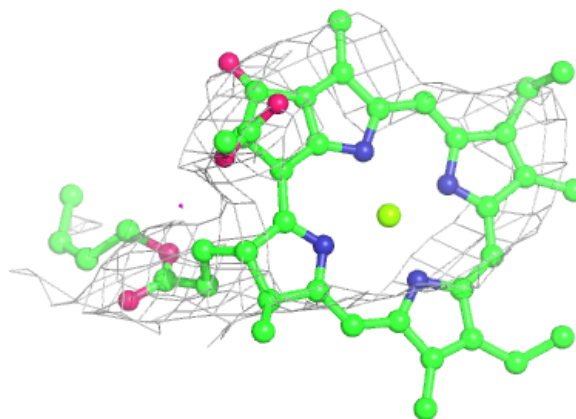
Electron density around CLA 4 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

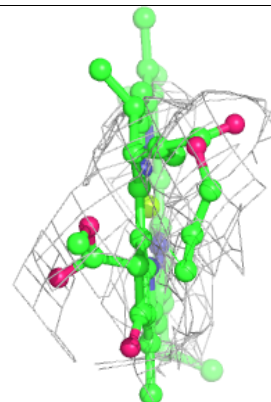
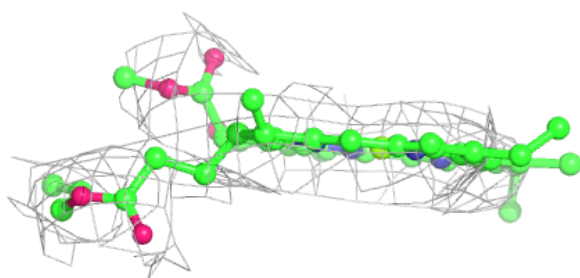
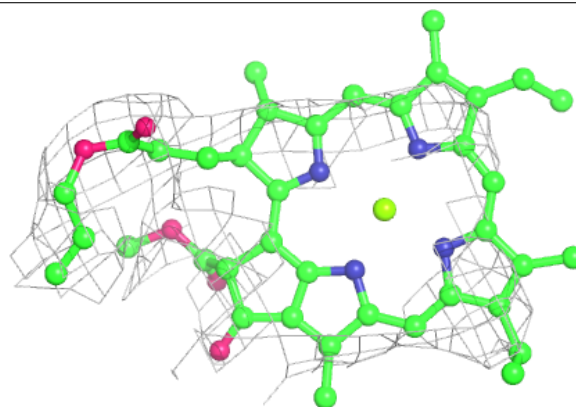


Electron density around CLA A 1137:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

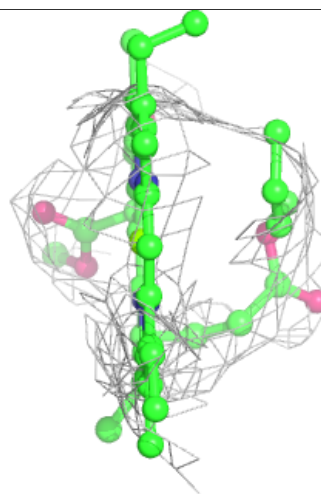
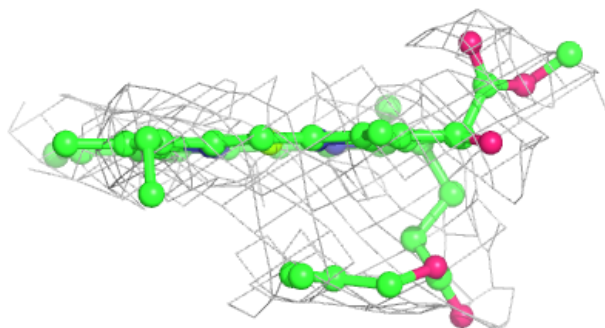
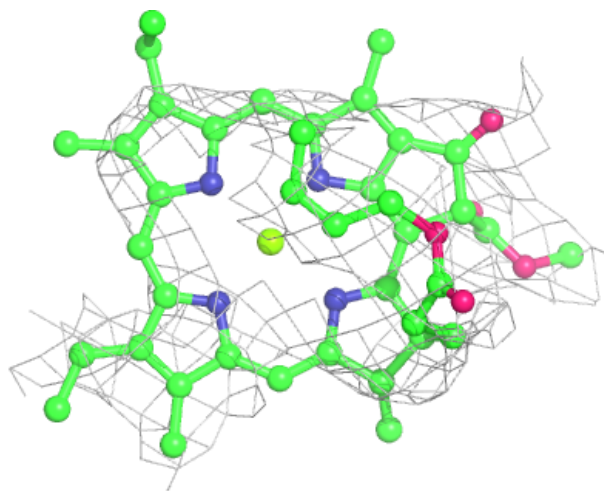
**Electron density around CLA A 1123:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



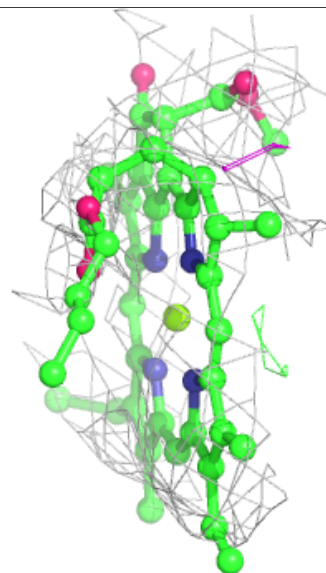
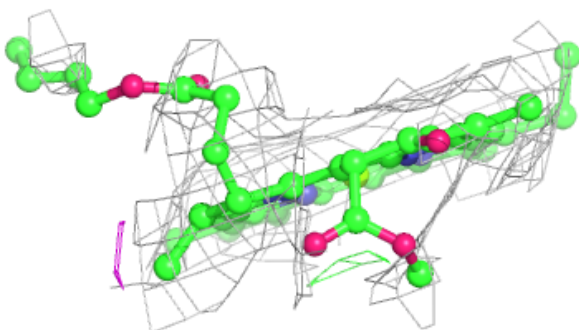
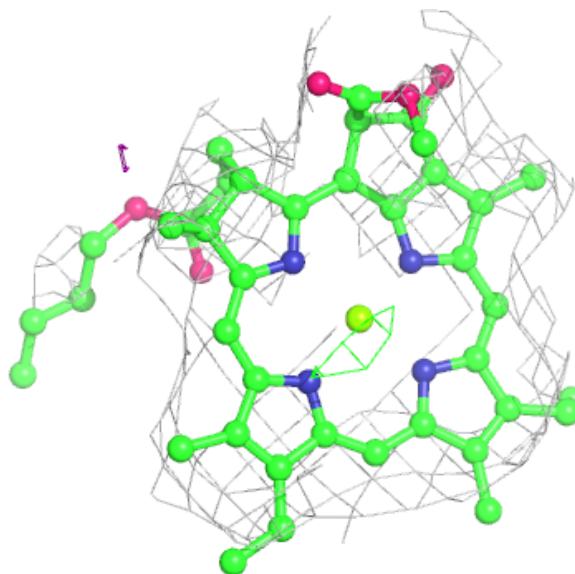
Electron density around CLA A 1136:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



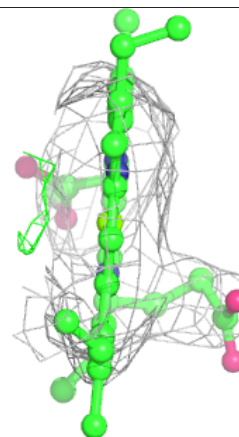
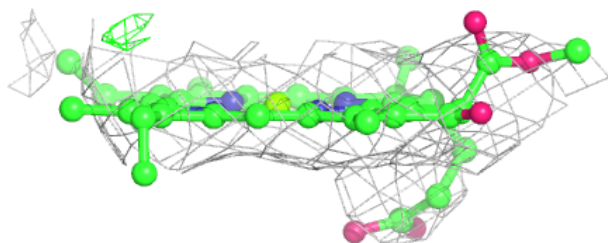
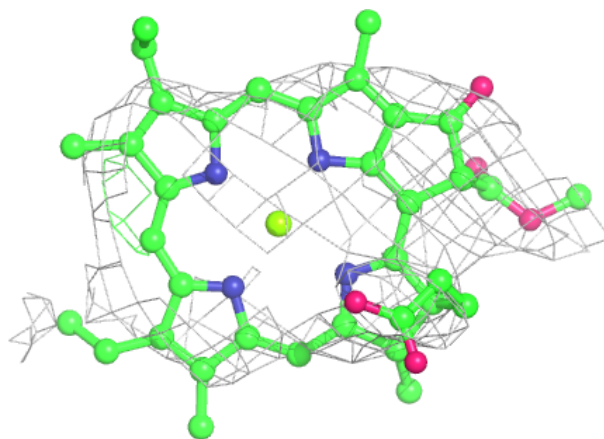
Electron density around CLA 2 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



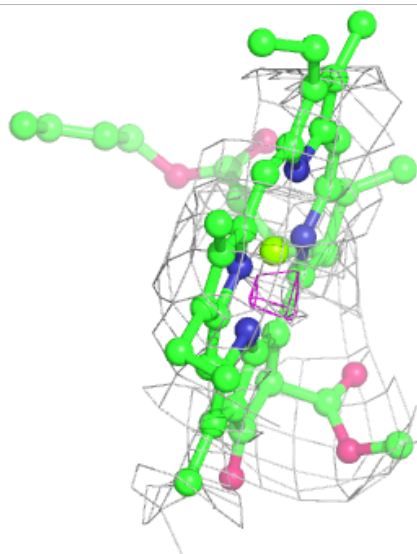
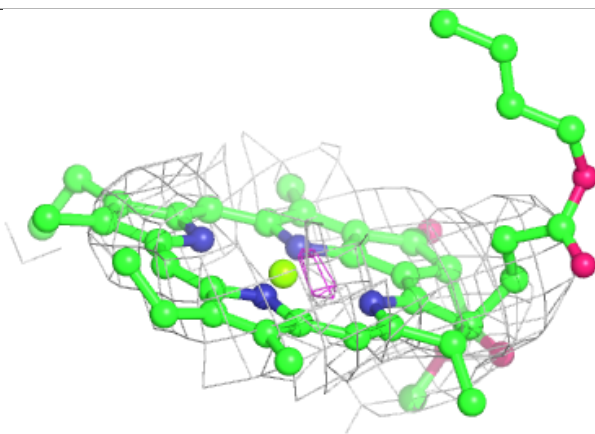
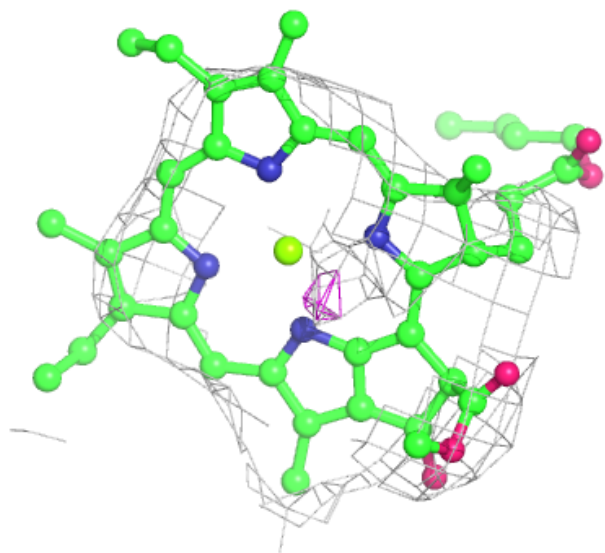
Electron density around CLA A 1113:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



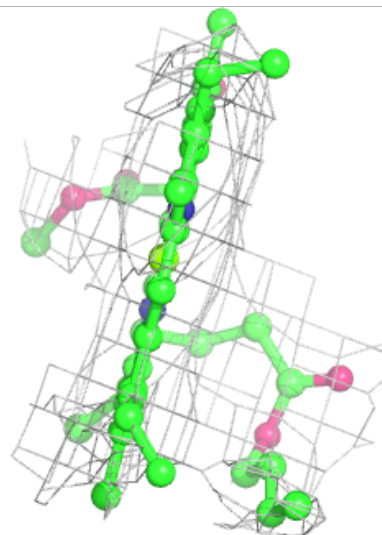
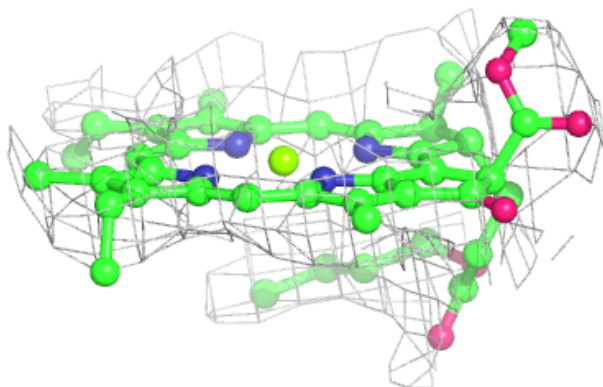
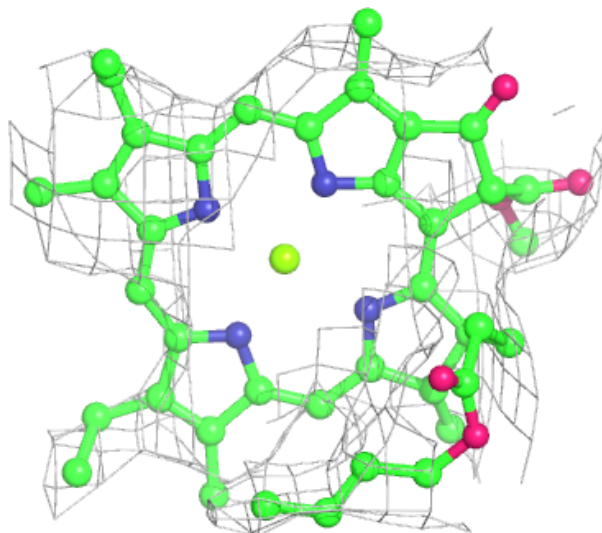
Electron density around CLA A 1118:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



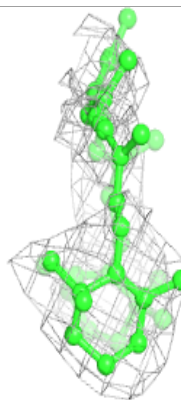
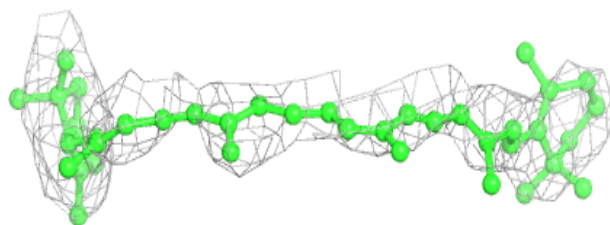
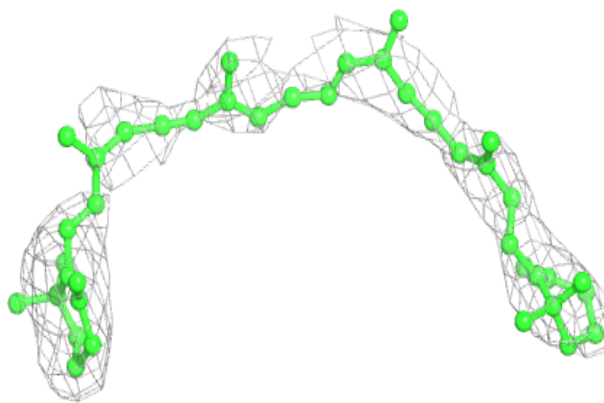
Electron density around CLA 2 604:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



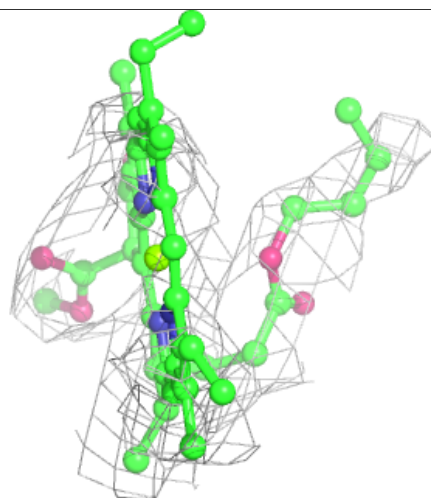
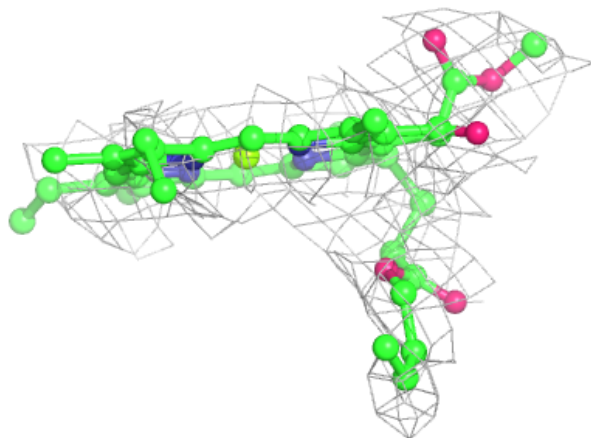
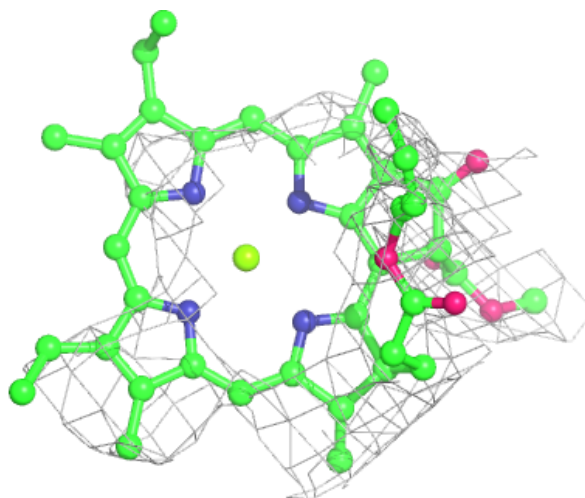
Electron density around BCR F 4002:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



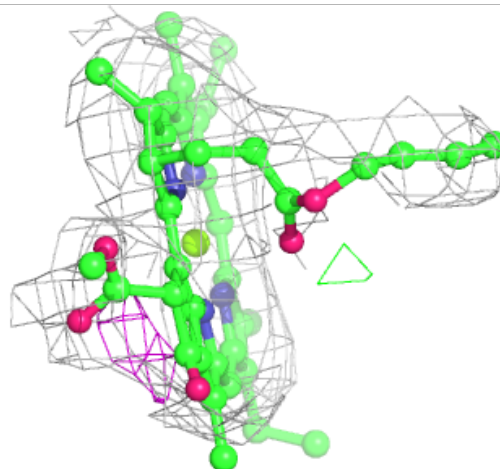
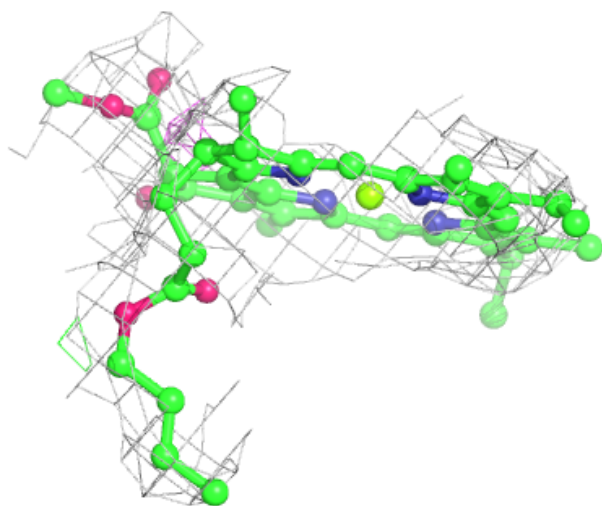
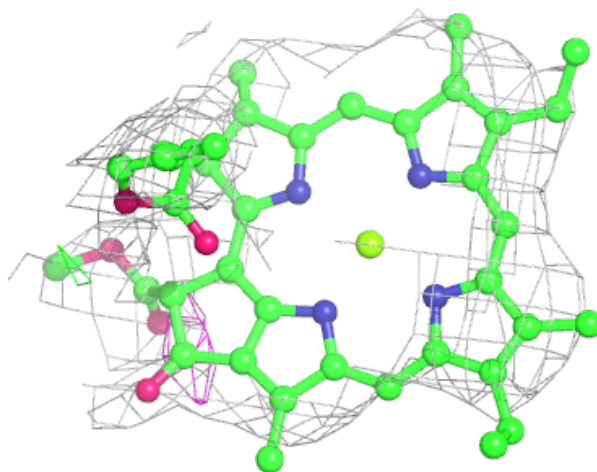
Electron density around CLA B 1213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



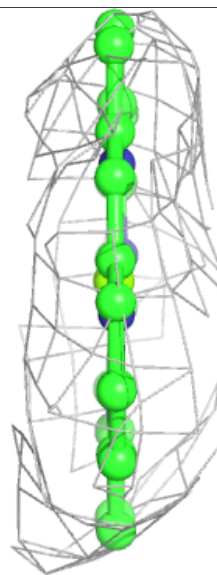
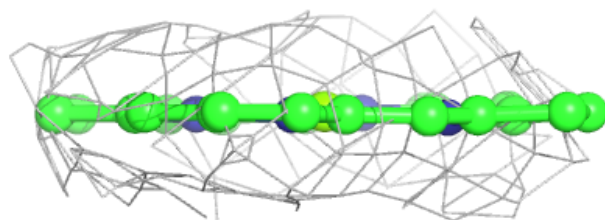
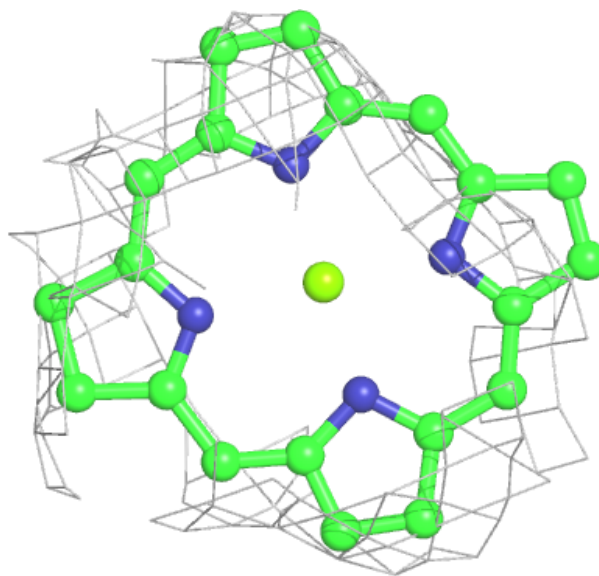
Electron density around CLA F 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



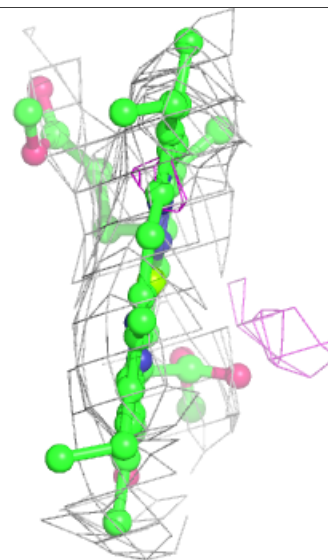
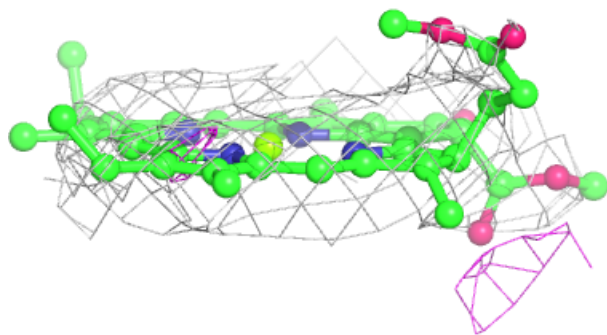
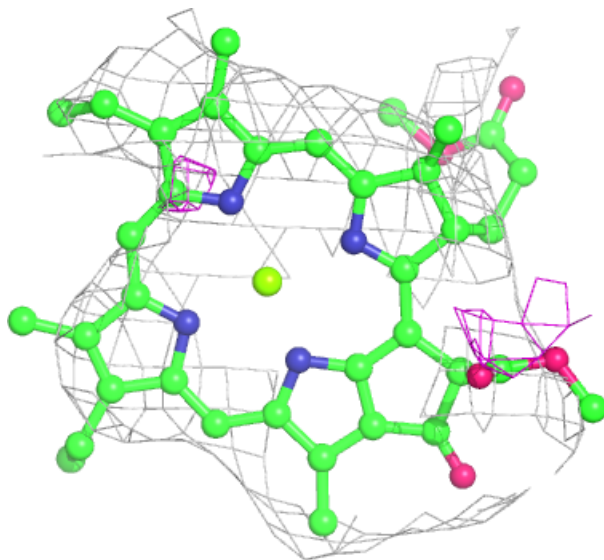
Electron density around CLA B 1207:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



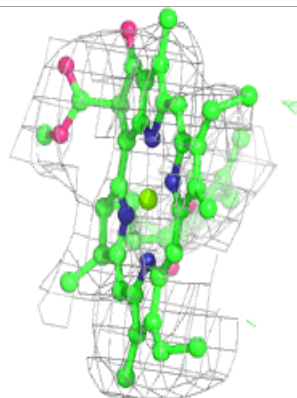
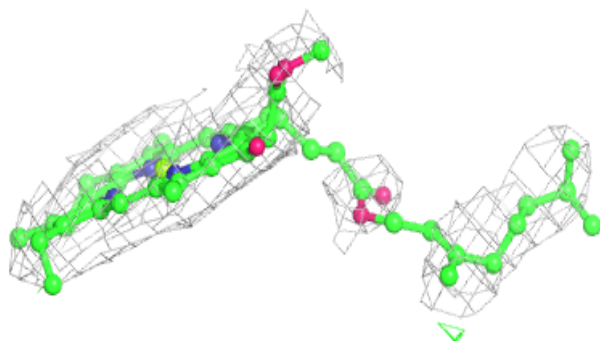
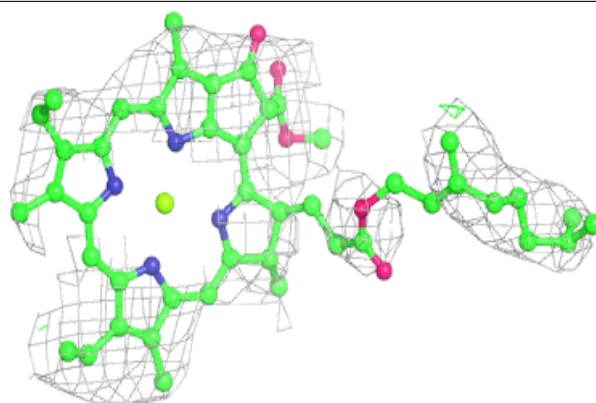
Electron density around CLA 1 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

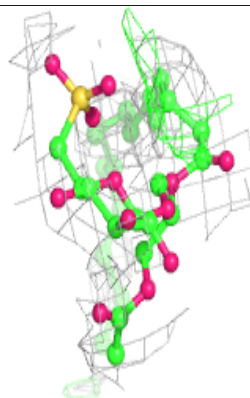
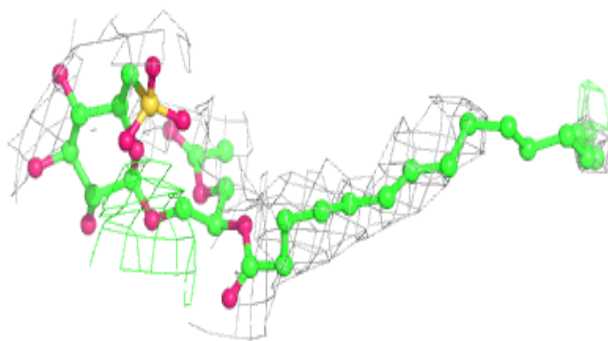
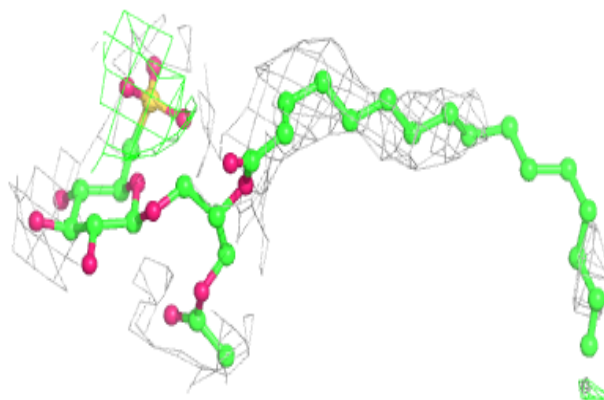


Electron density around CLA B 1220:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

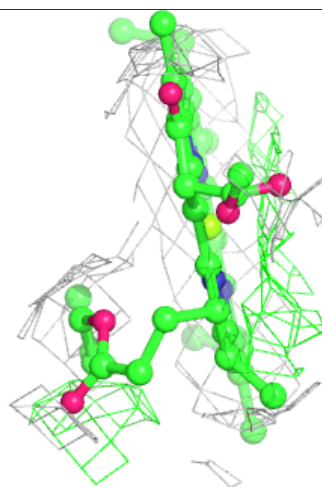
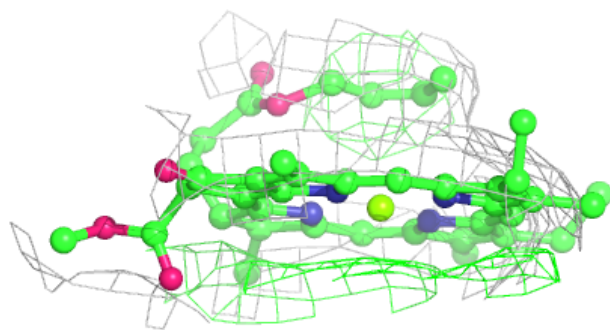
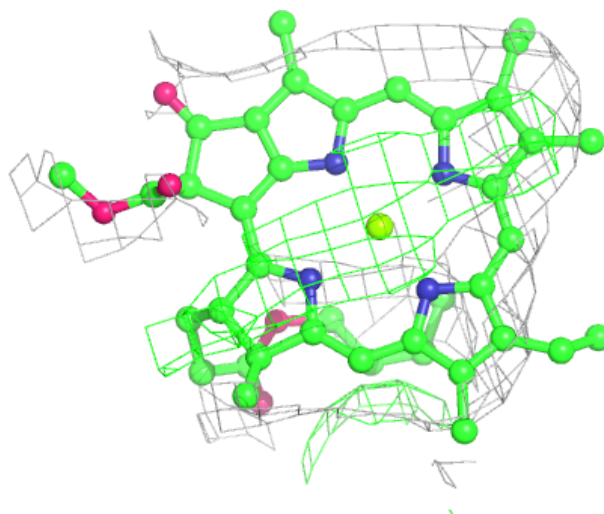
**Electron density around SQD 1 811:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



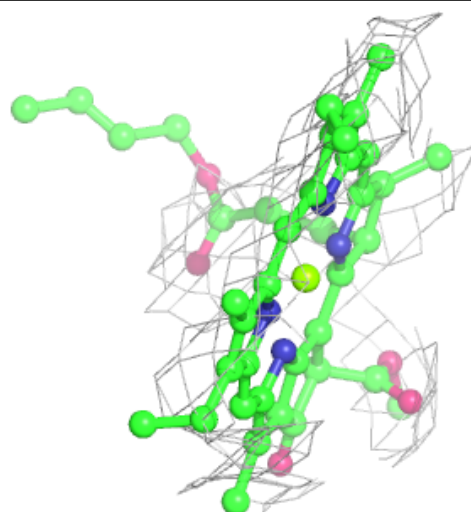
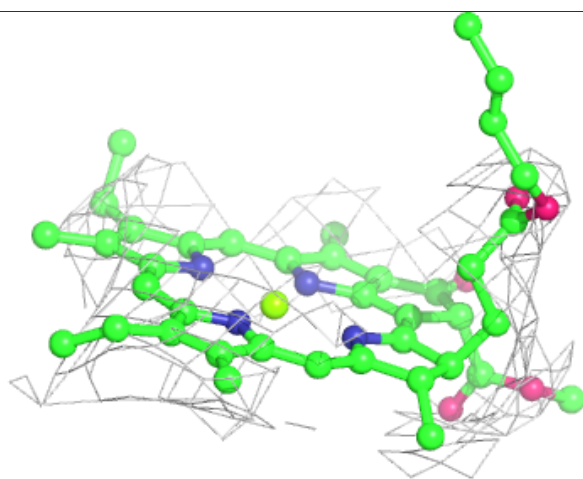
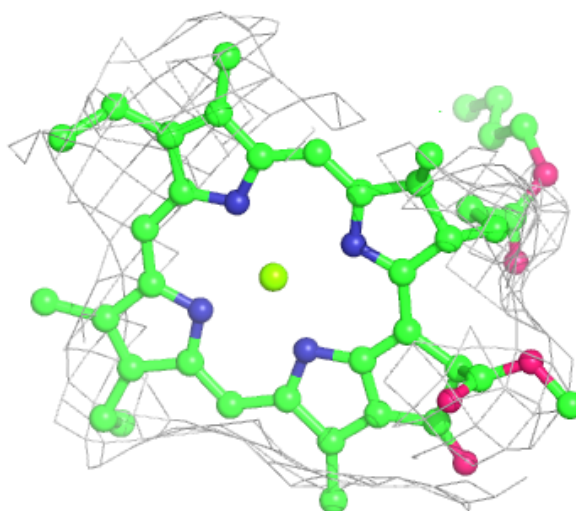
Electron density around CLA 3 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



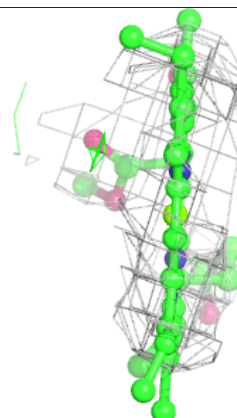
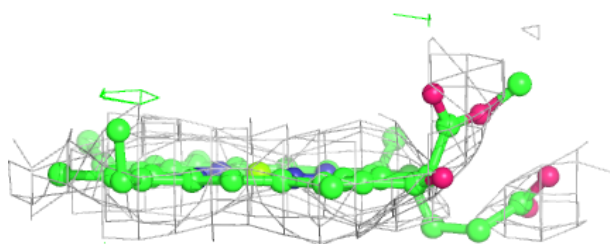
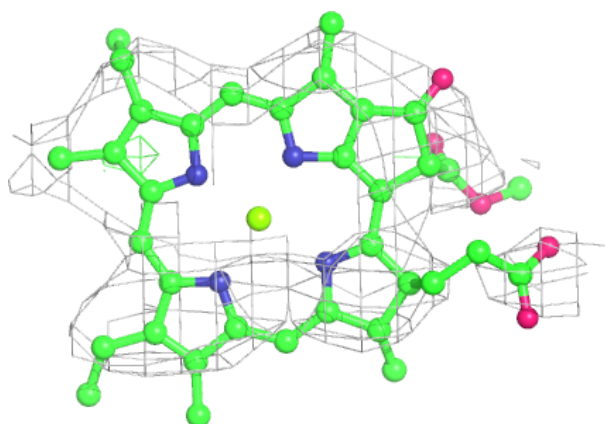
Electron density around CLA A 1133:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

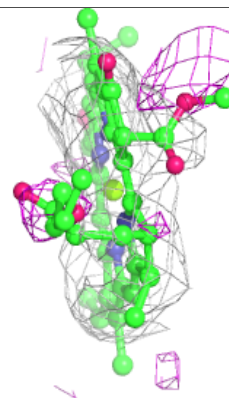
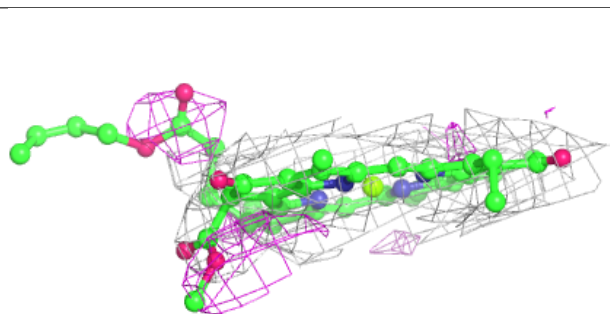
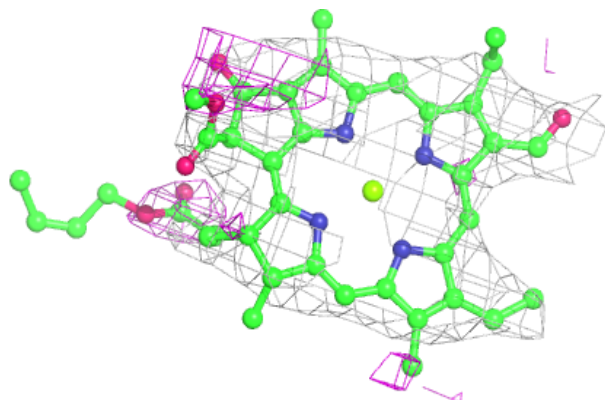


Electron density around CLA A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

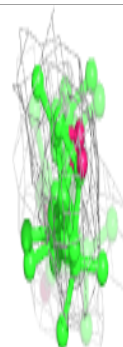
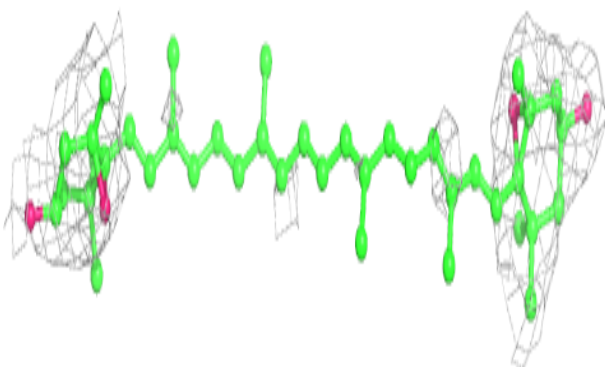
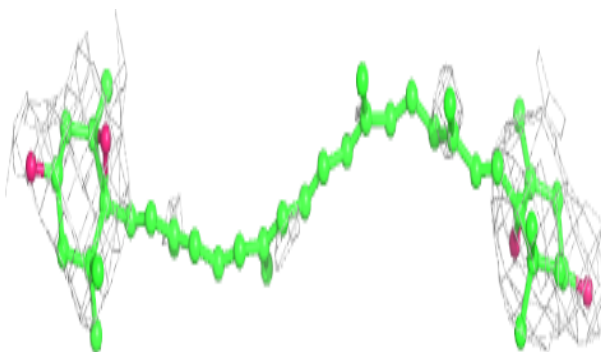
**Electron density around CHL 4 613:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



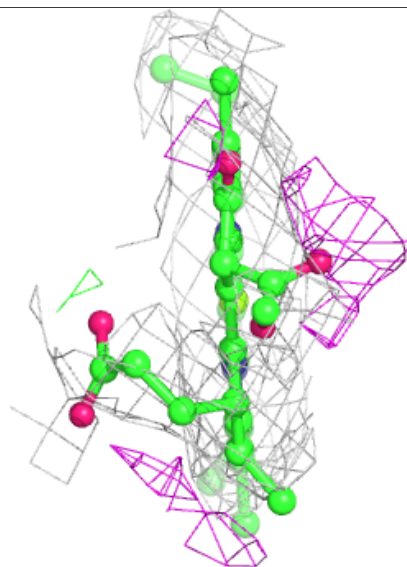
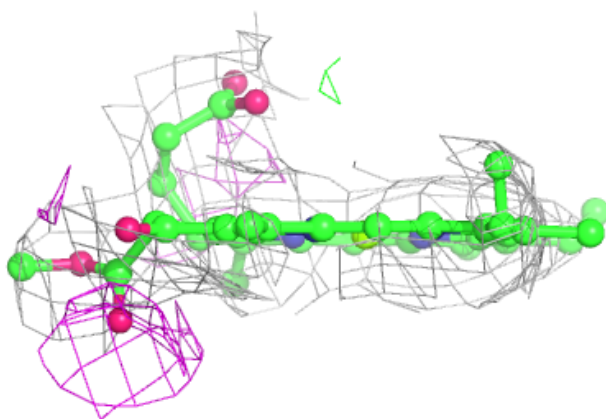
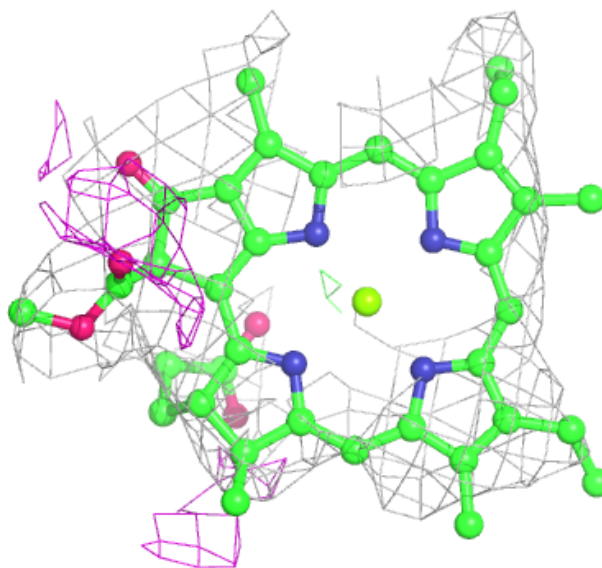
Electron density around XAT 1 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



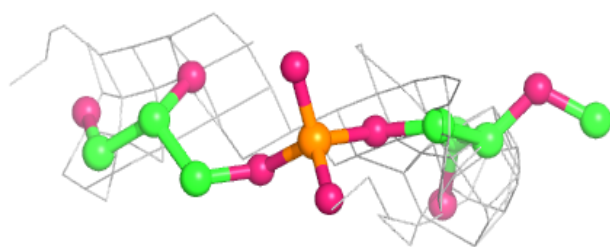
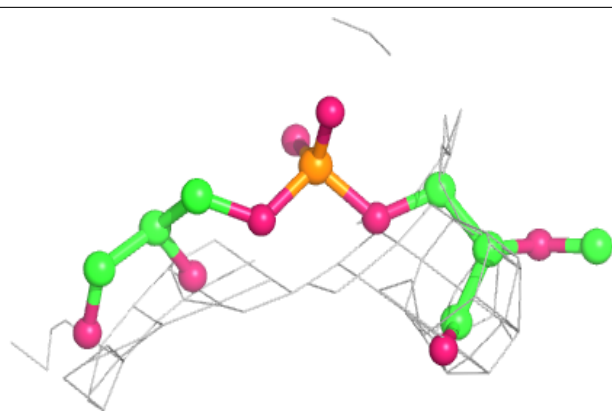
Electron density around CLA 1 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

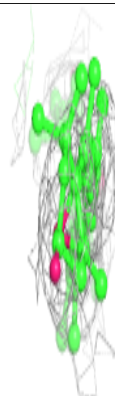
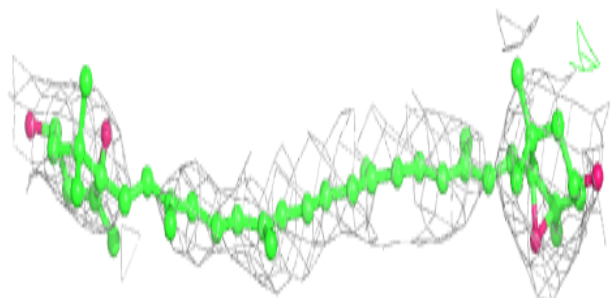
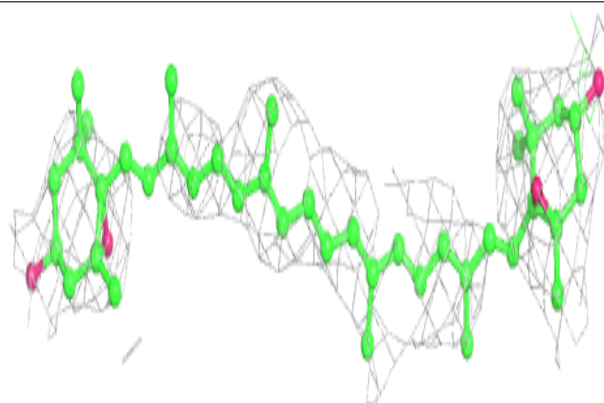


Electron density around LHG A 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

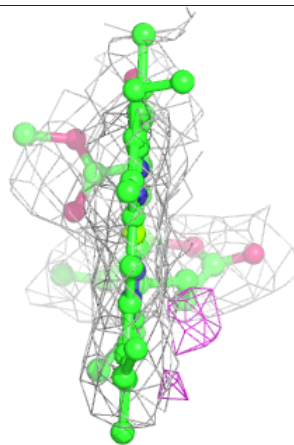
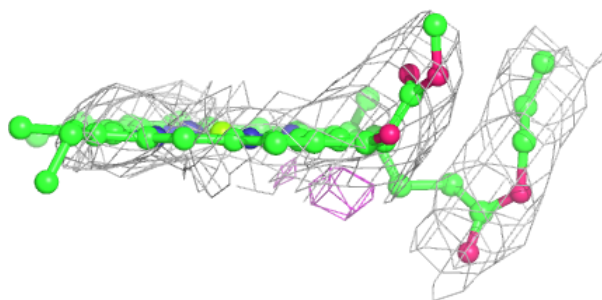
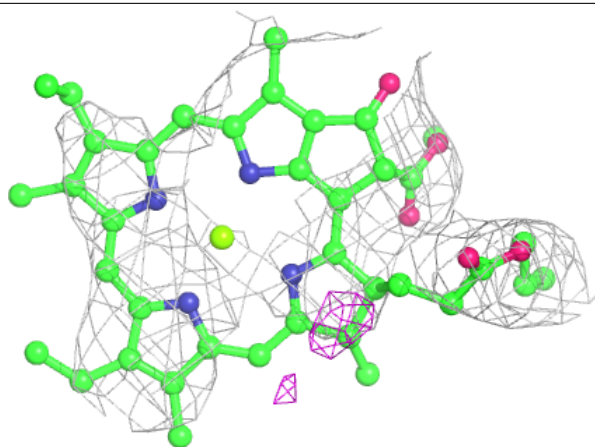
**Electron density around XAT 2 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



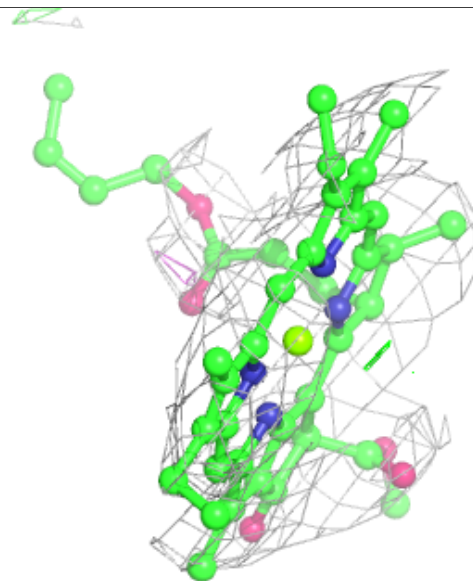
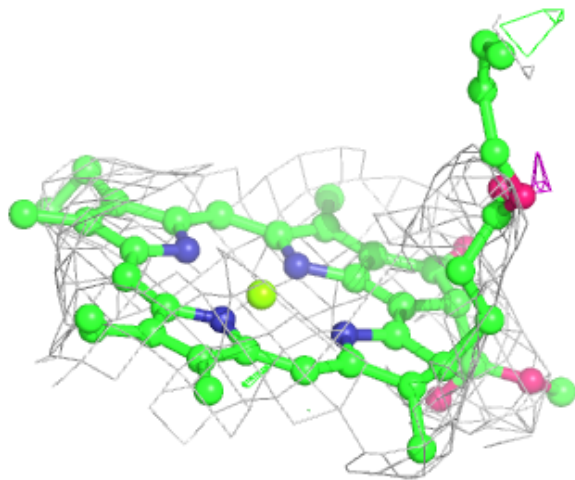
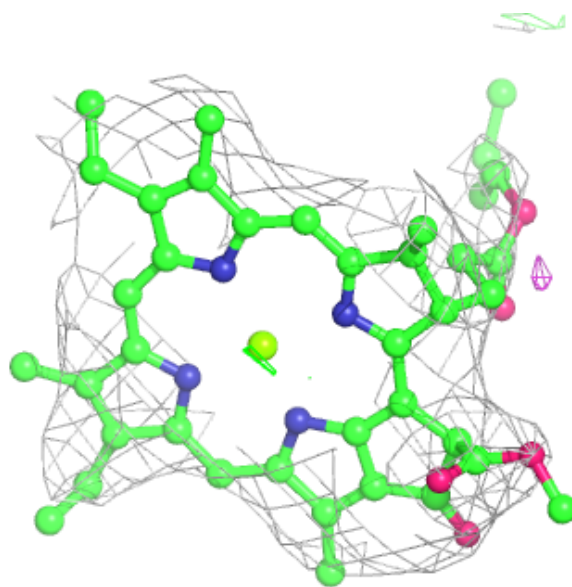
Electron density around CLA 1 605:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



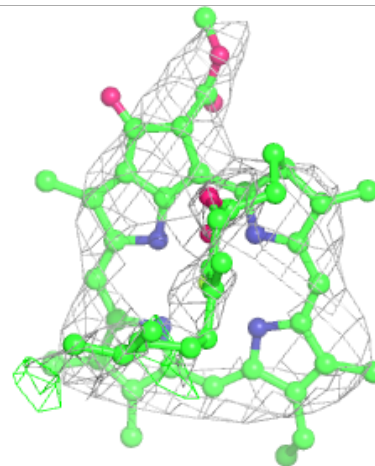
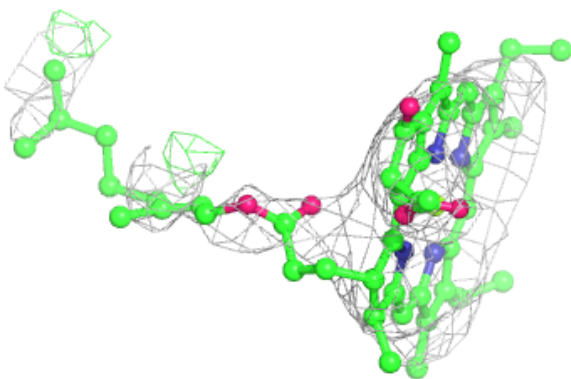
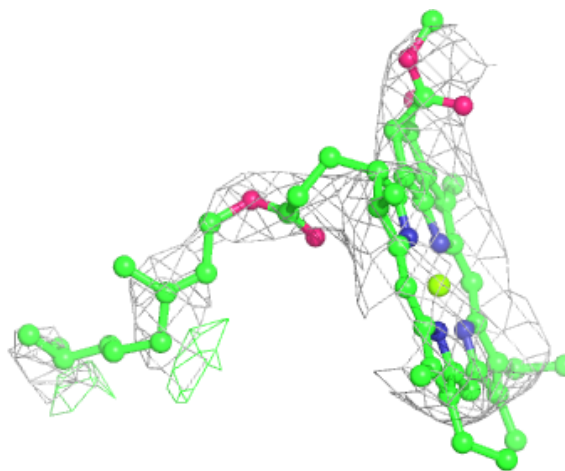
Electron density around CLA B 1232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



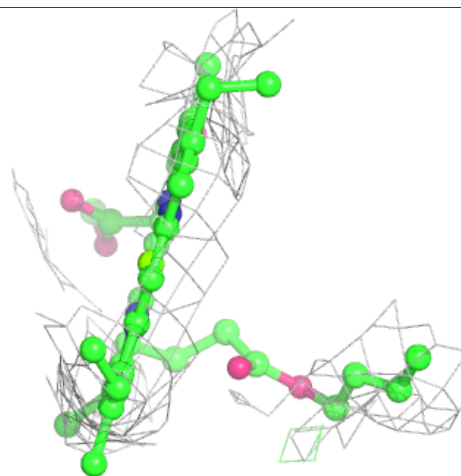
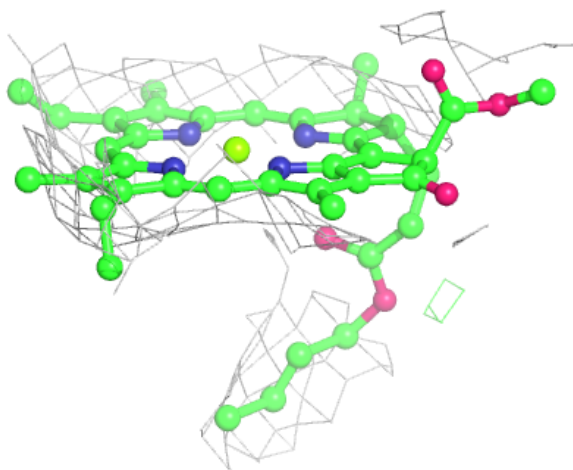
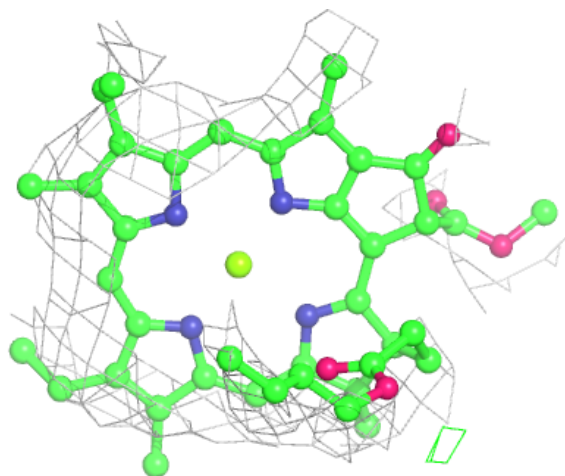
Electron density around CLA A 1140:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



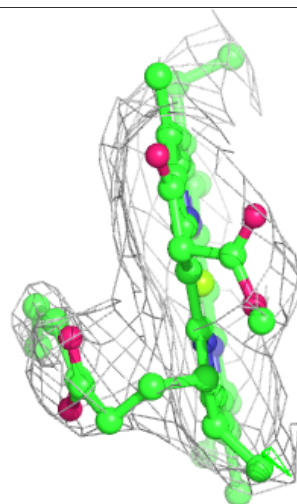
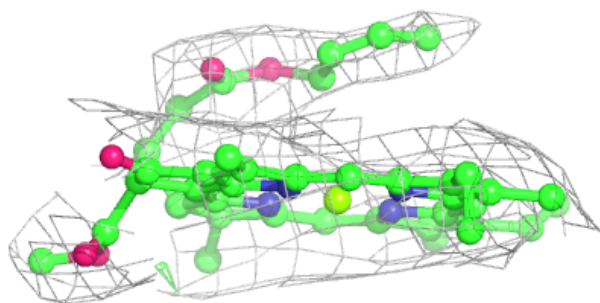
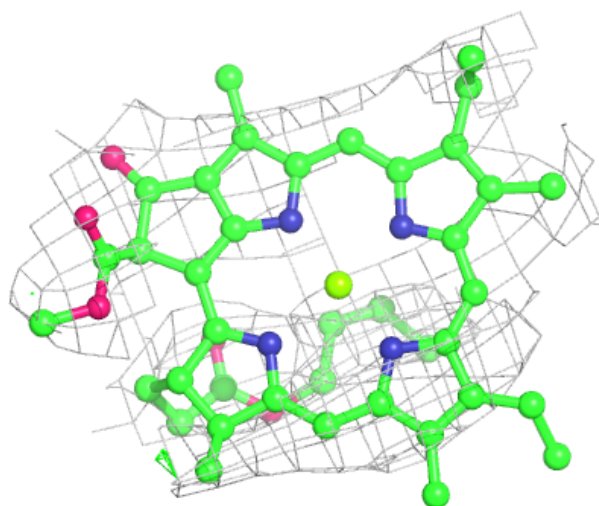
Electron density around CLA A 1109:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



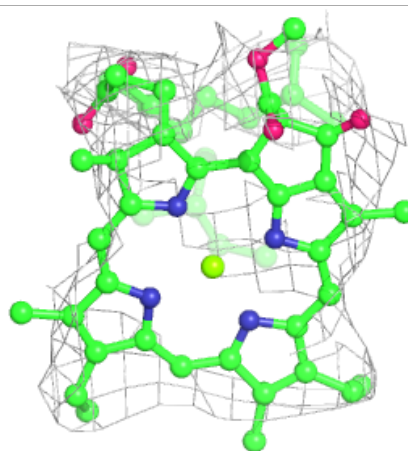
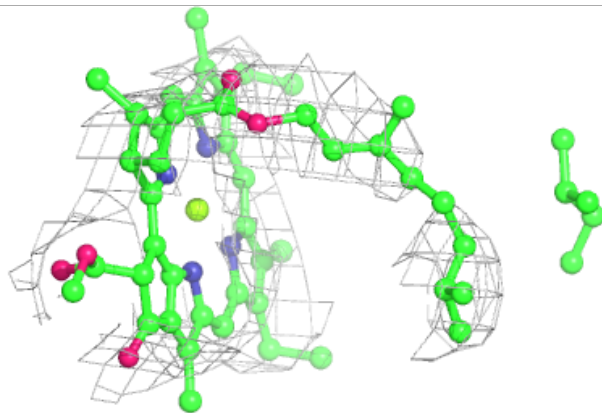
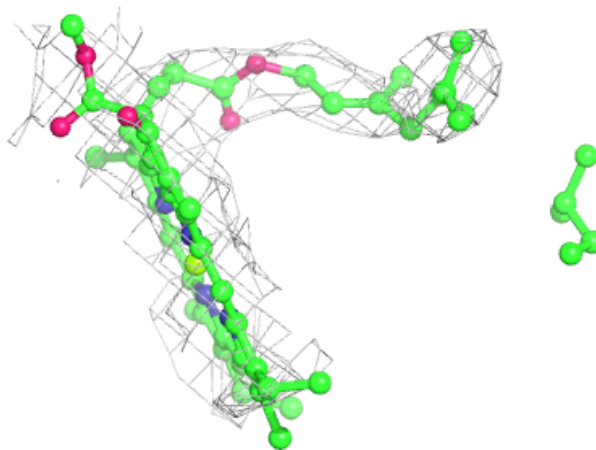
Electron density around CLA B 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



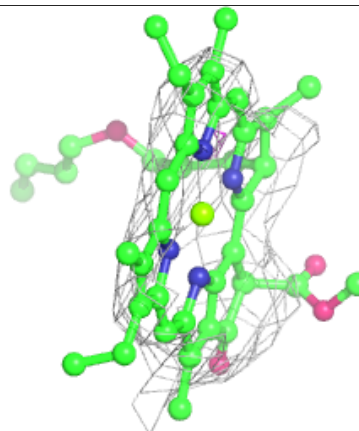
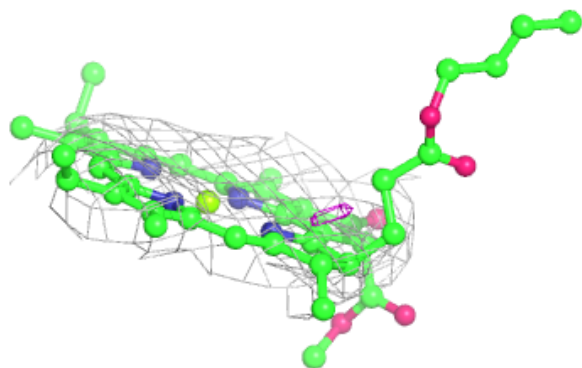
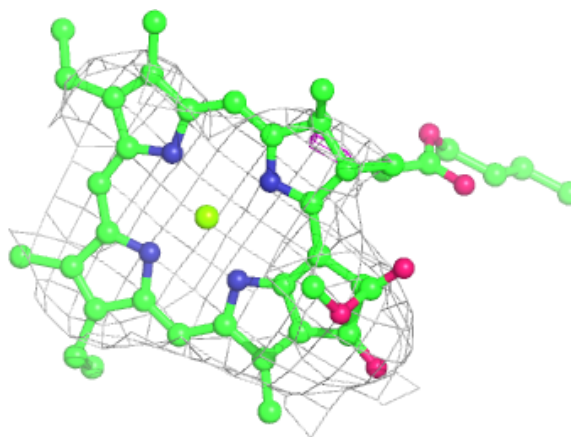
Electron density around CLA 1 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

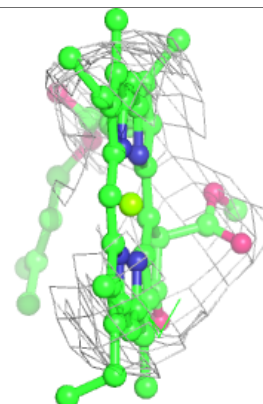
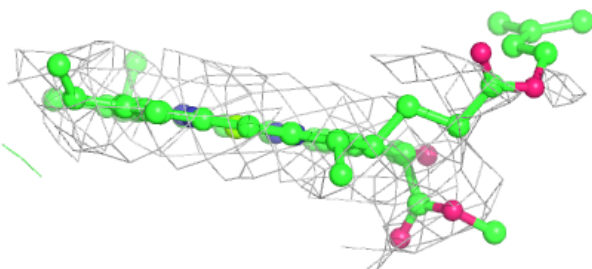
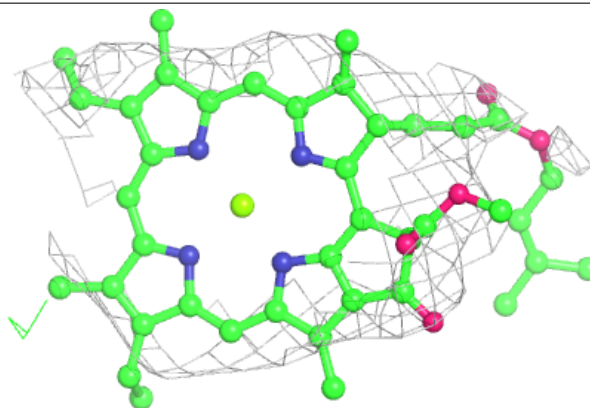


Electron density around CLA A 1112:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

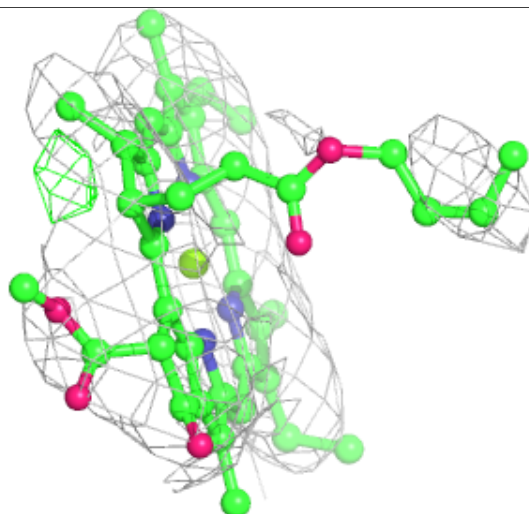
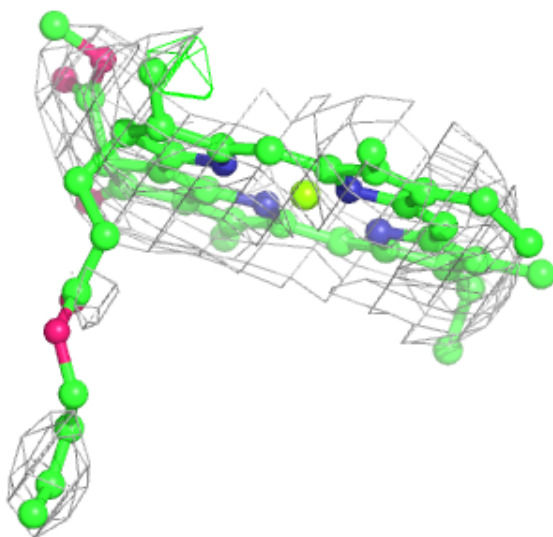
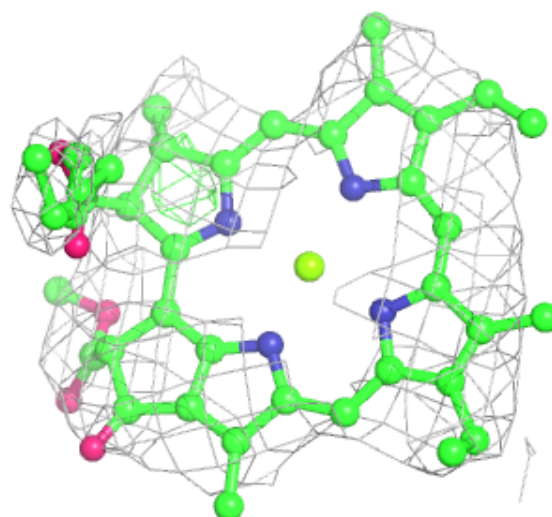
**Electron density around CLA 2 615:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



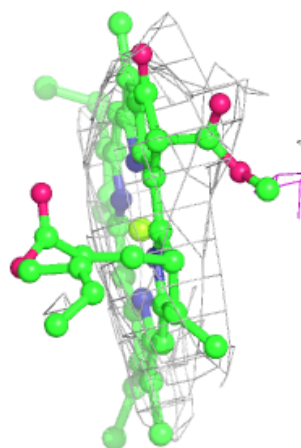
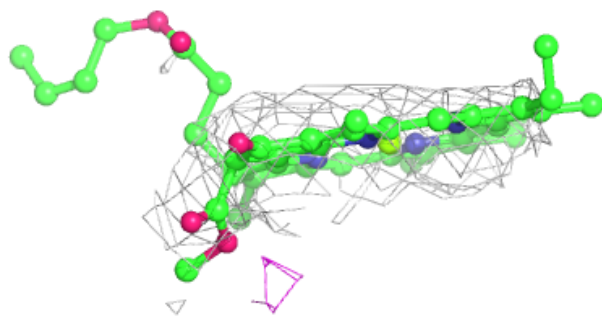
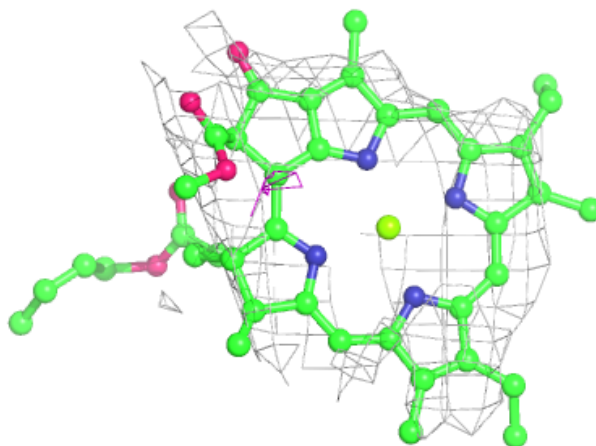
Electron density around CLA B 1225:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



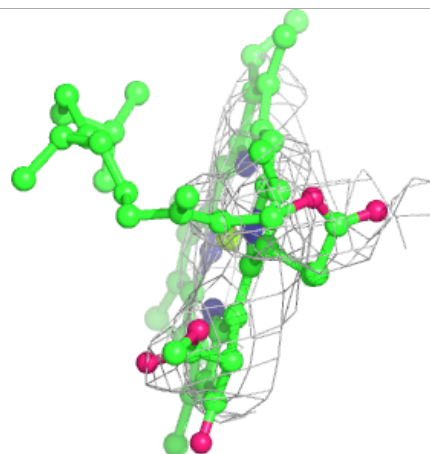
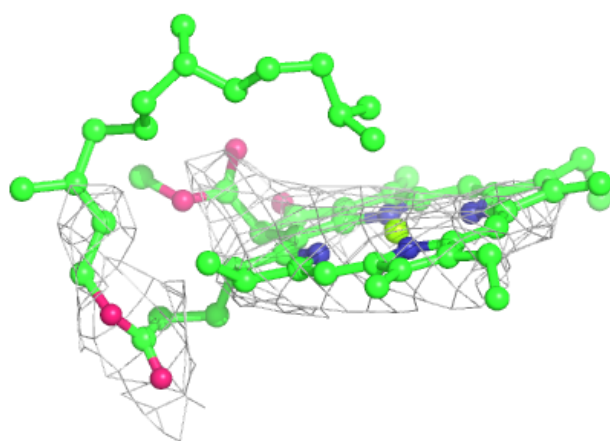
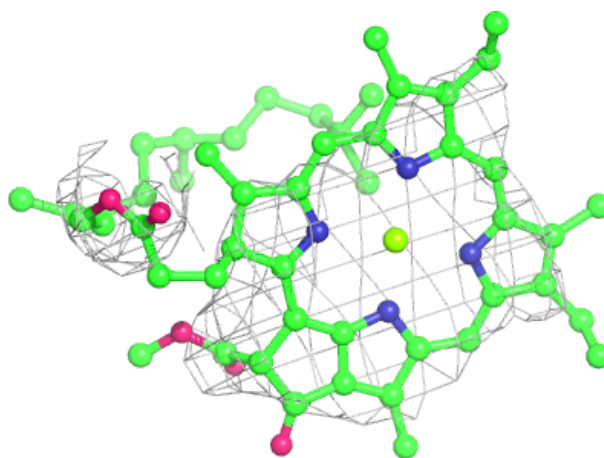
Electron density around CLA A 1132:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



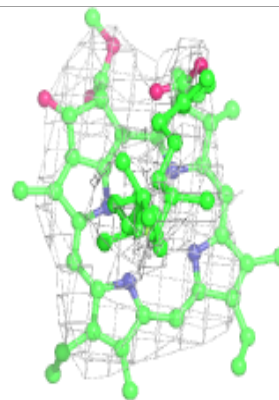
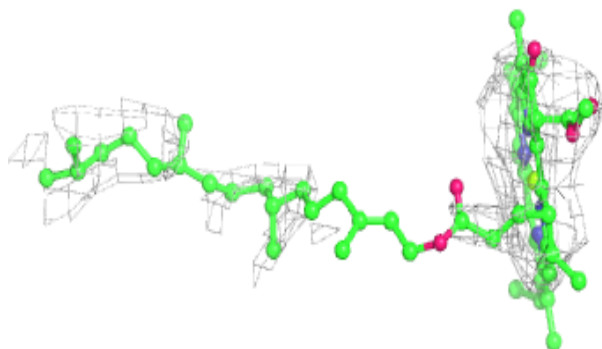
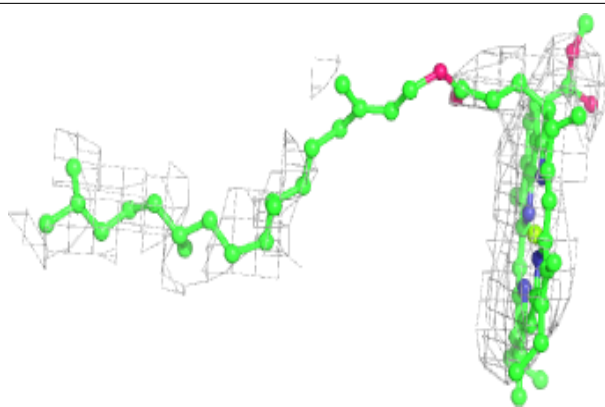
Electron density around CLA A 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



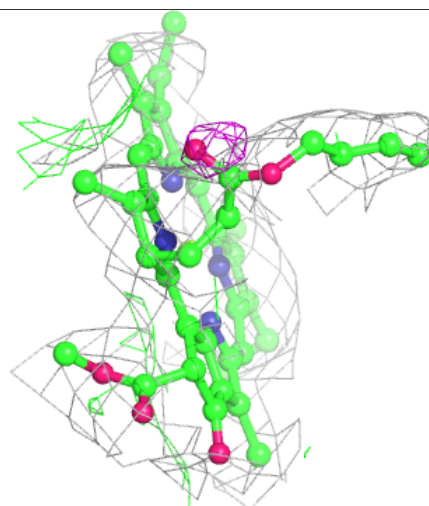
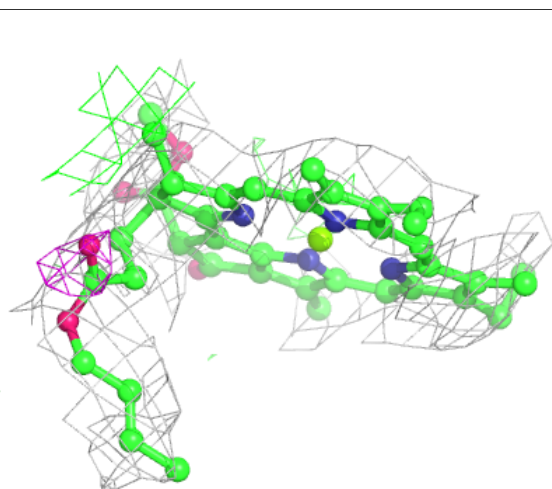
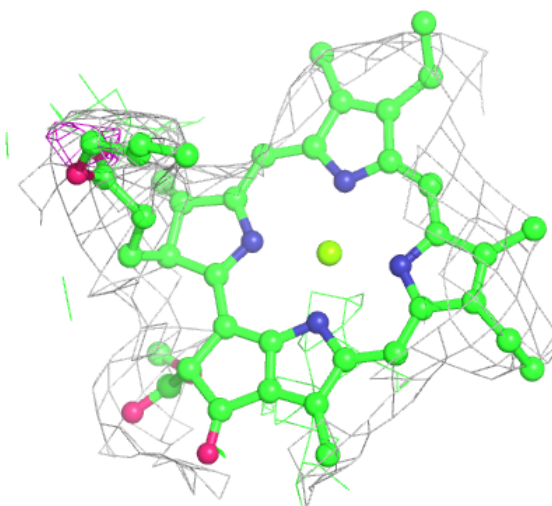
Electron density around CLA B 1239:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



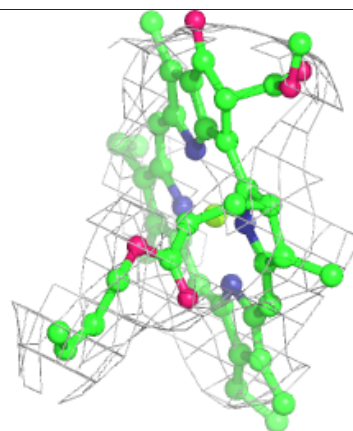
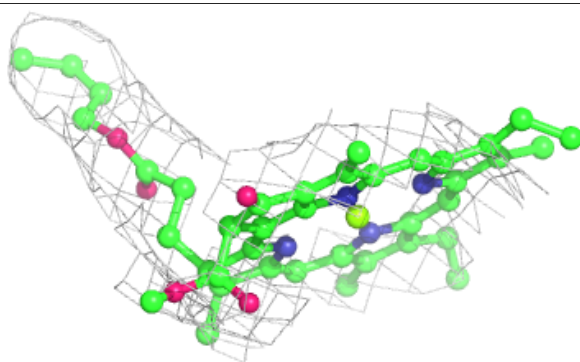
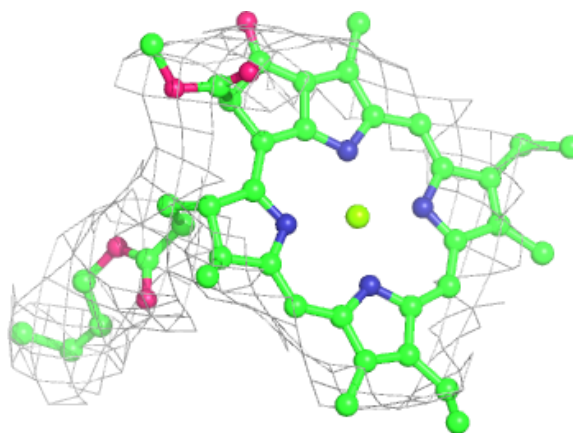
Electron density around CLA 4 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

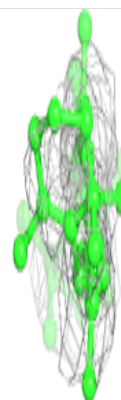
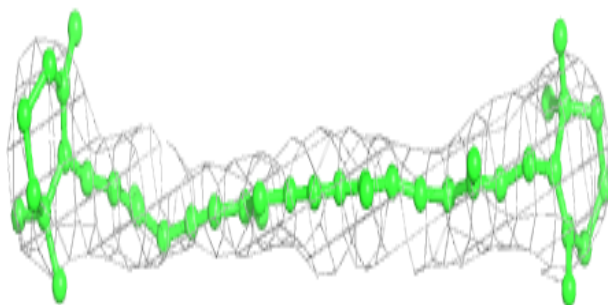
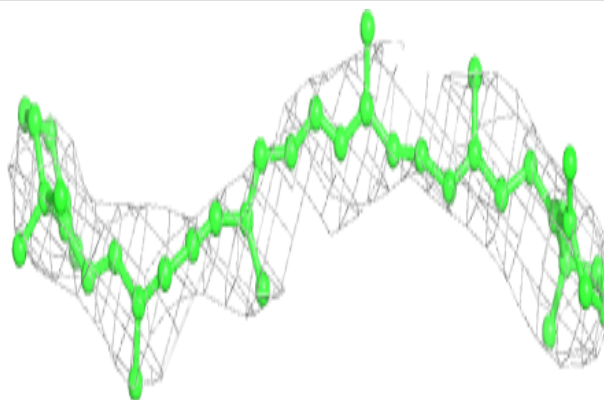


Electron density around CLA 1 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

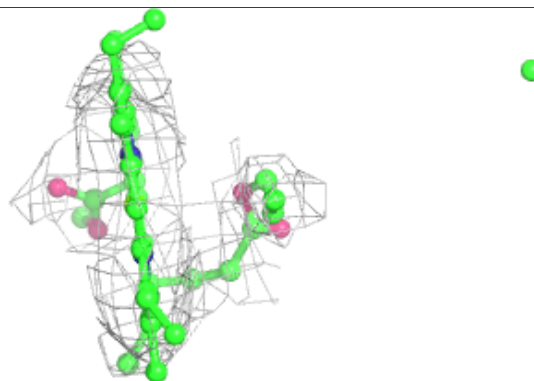
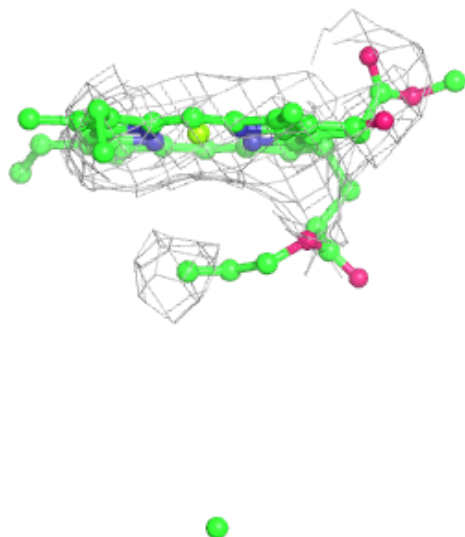
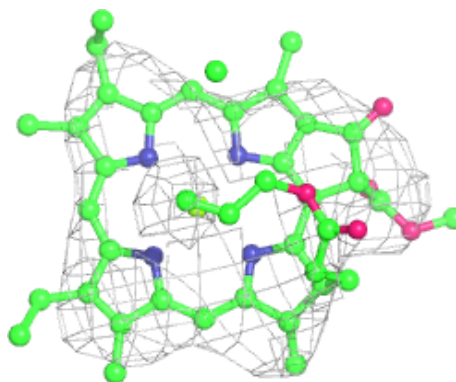
**Electron density around BCR B 4004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



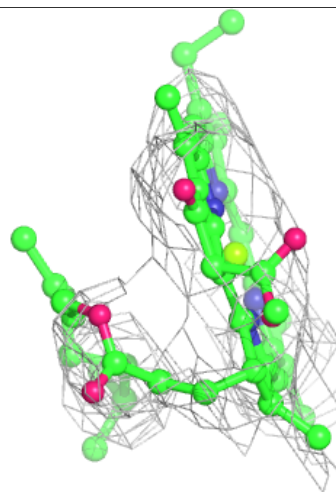
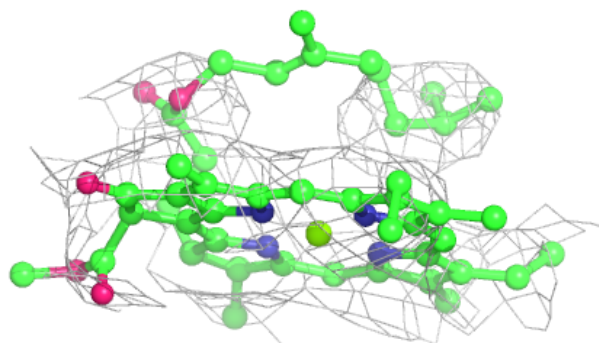
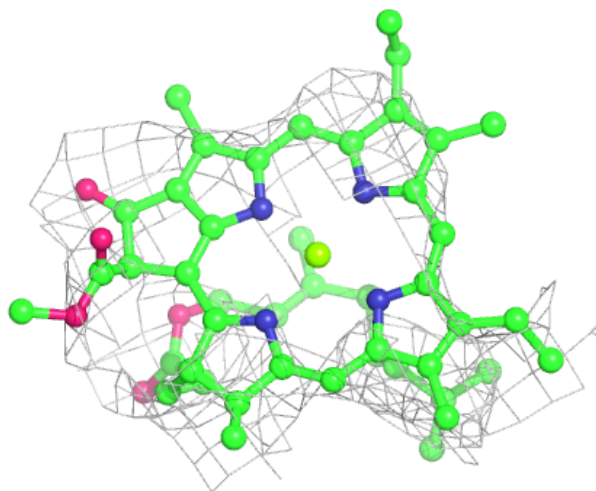
Electron density around CLA B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



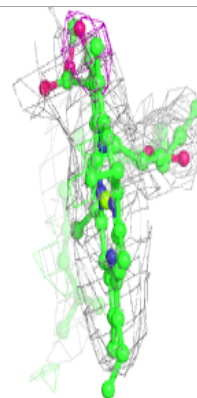
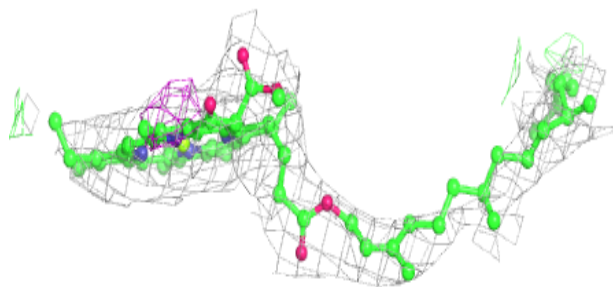
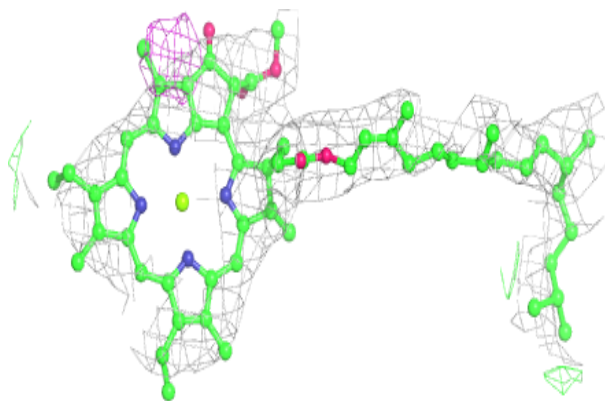
Electron density around CLA A 1130:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



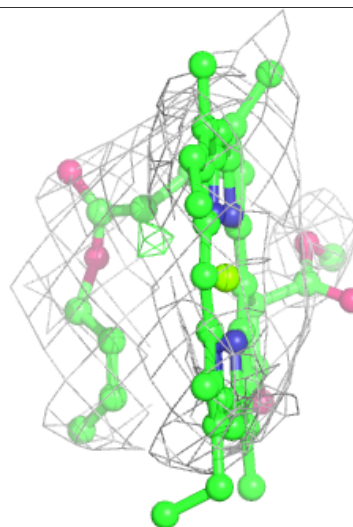
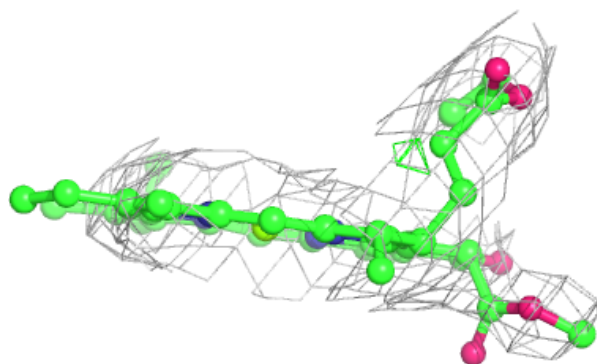
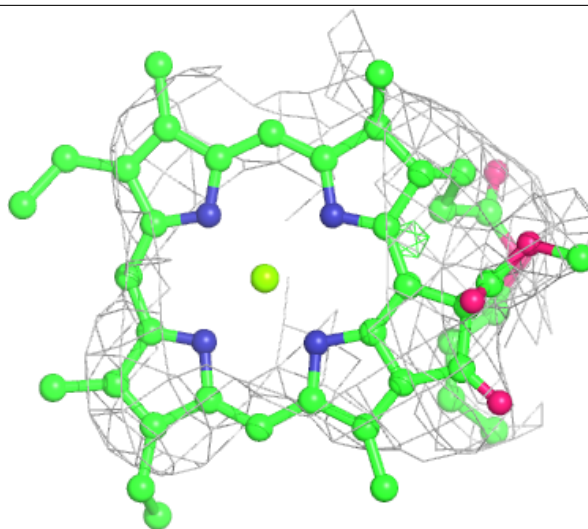
Electron density around CLA B 1240:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



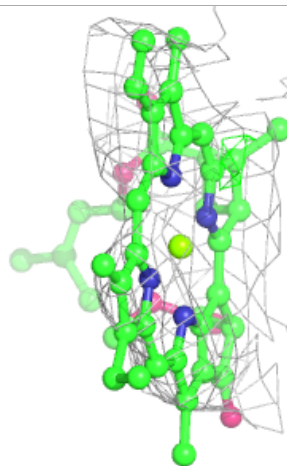
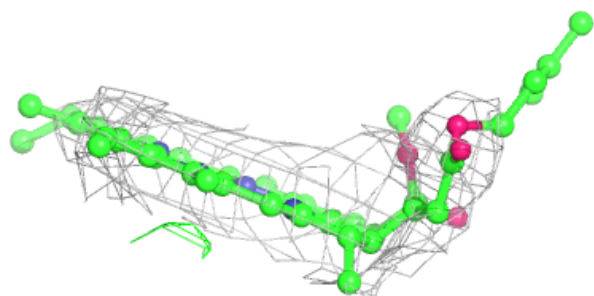
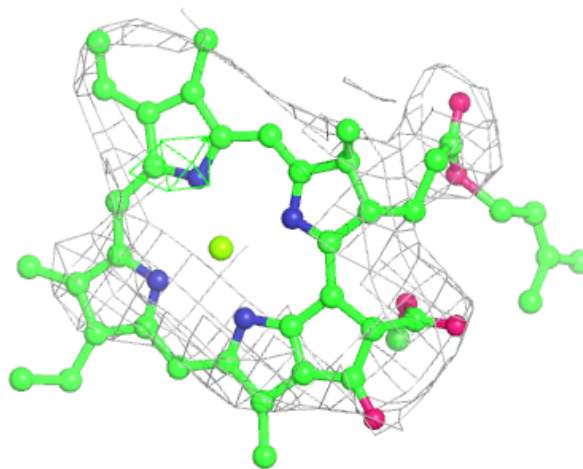
Electron density around CLA A 1127:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



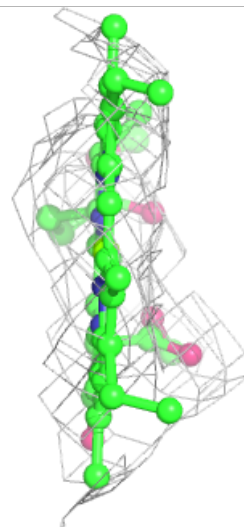
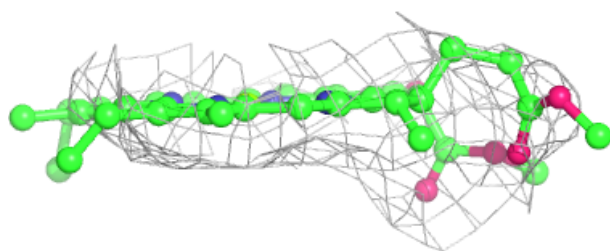
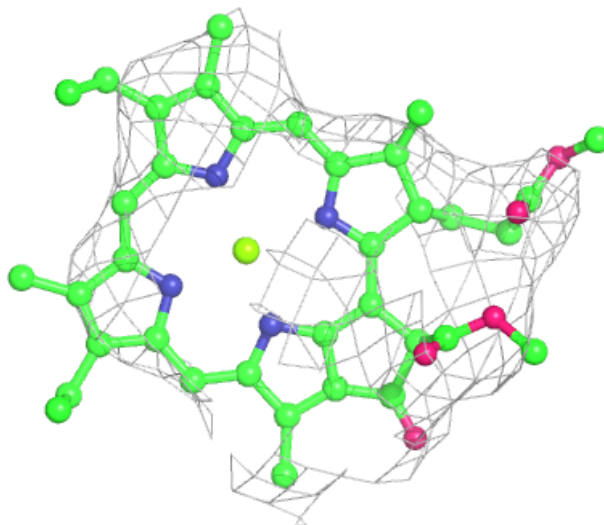
Electron density around CL0 A 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



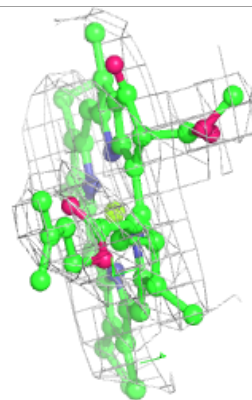
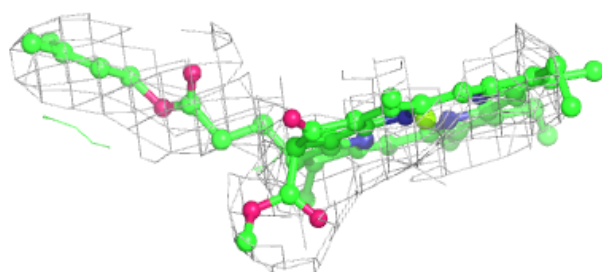
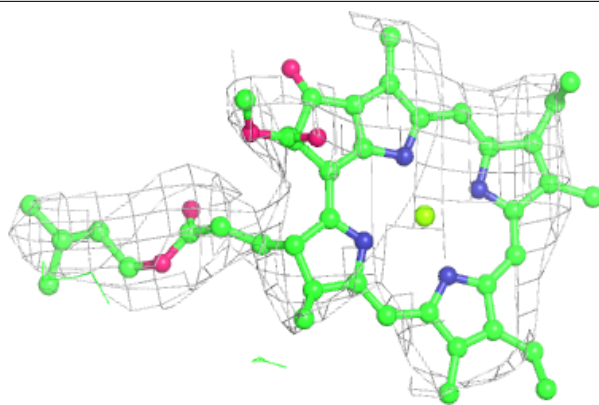
Electron density around CLA 1 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



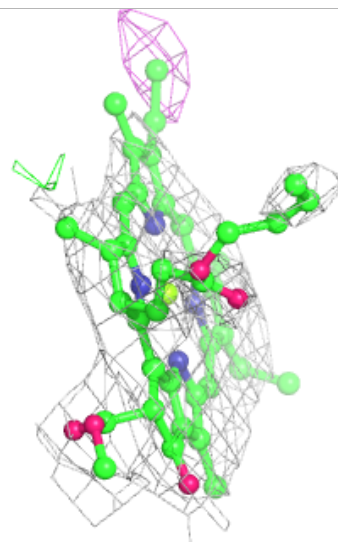
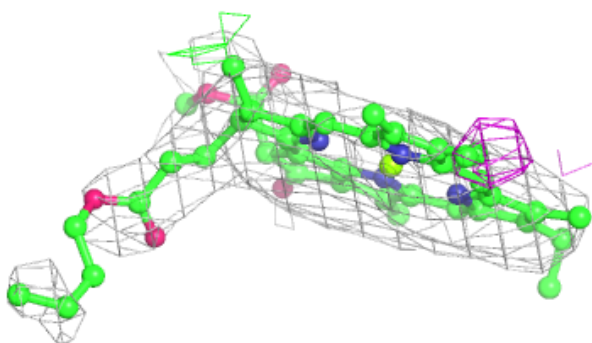
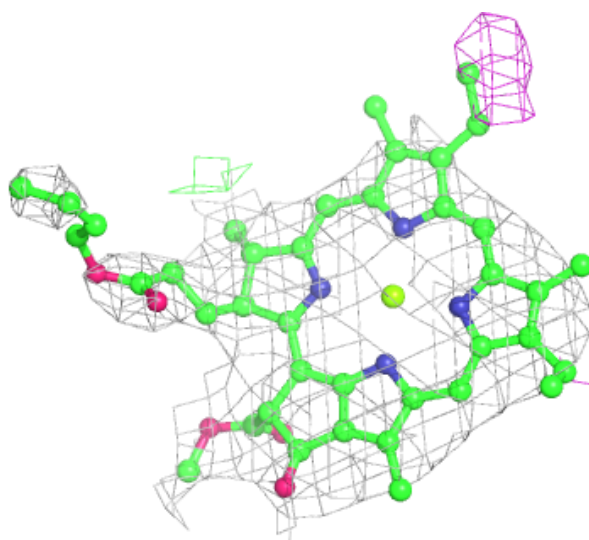
Electron density around CLA B 1223:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



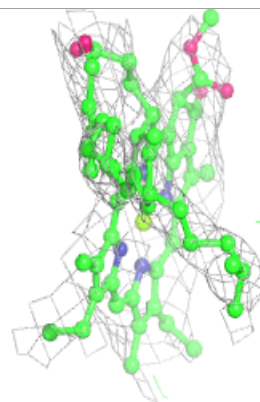
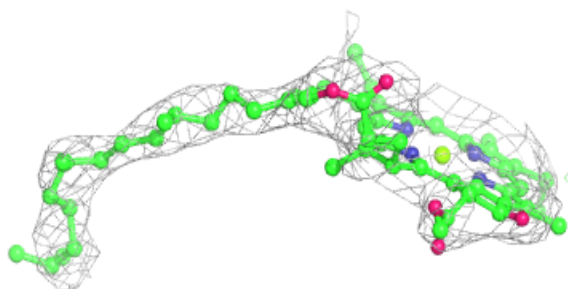
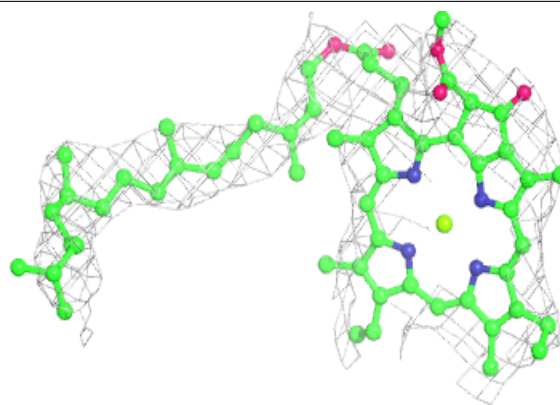
Electron density around CLA B 1230:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

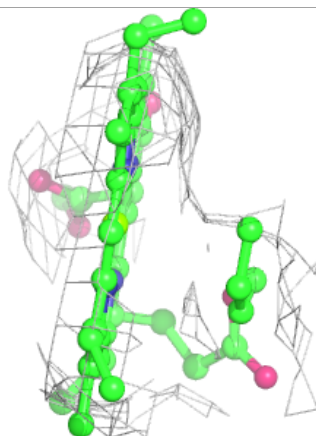
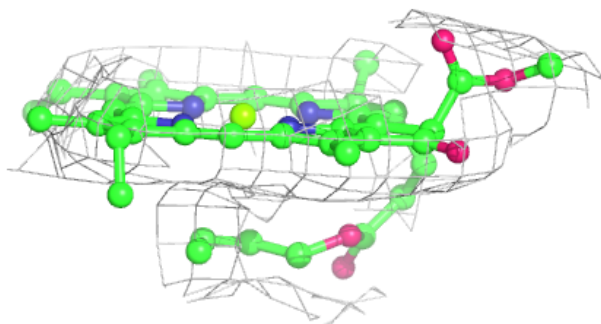
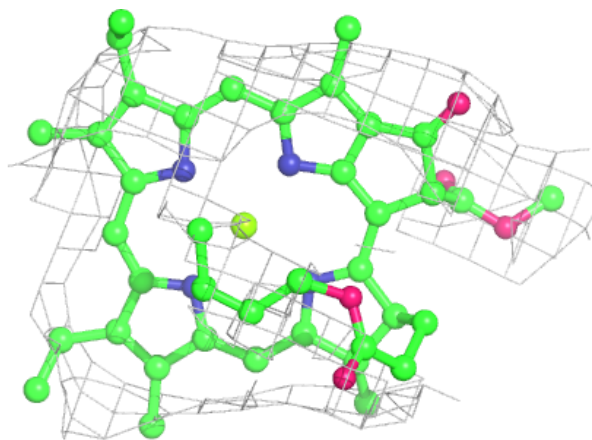


Electron density around CLA A 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

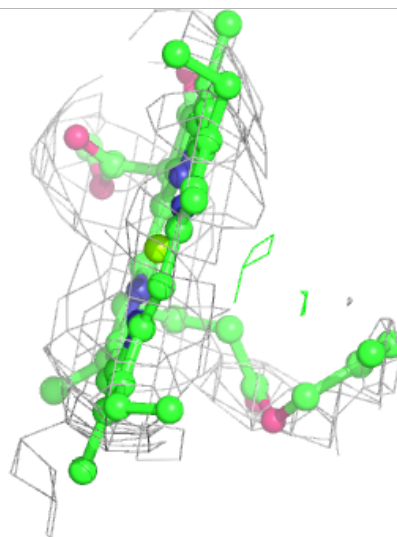
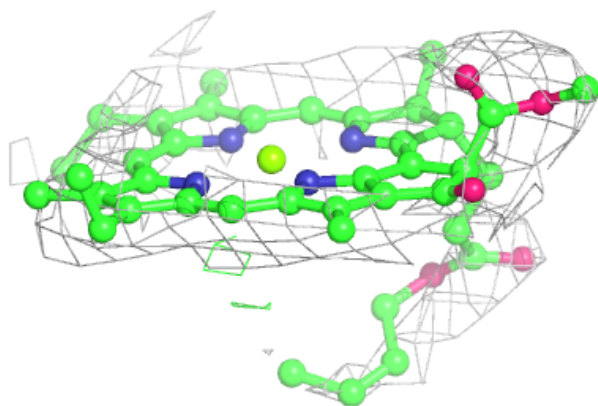
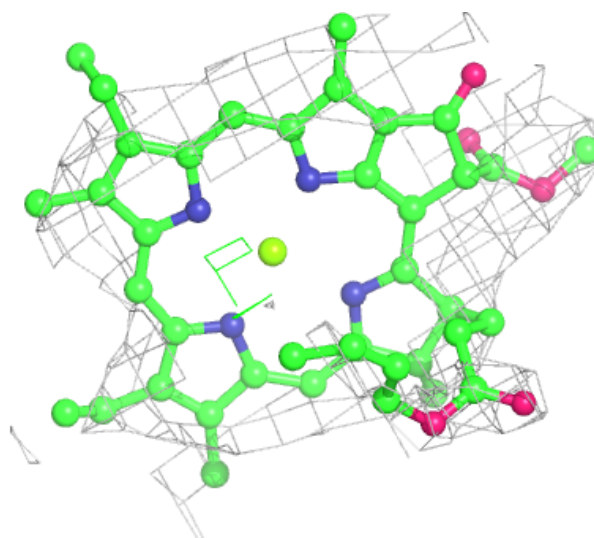
**Electron density around CLA B 1237:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



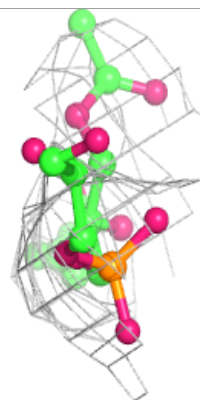
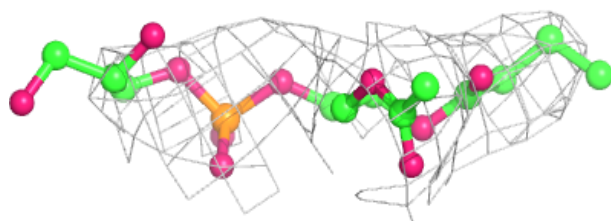
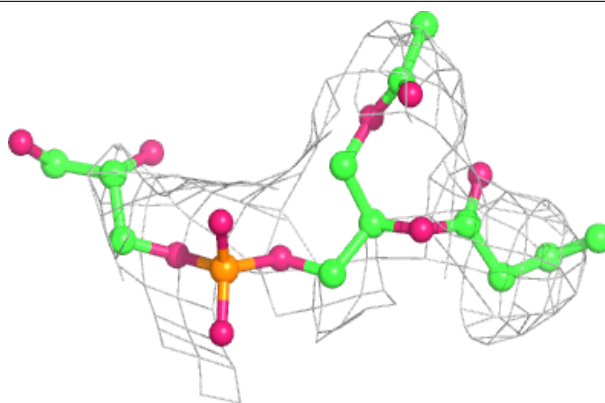
Electron density around CLA B 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



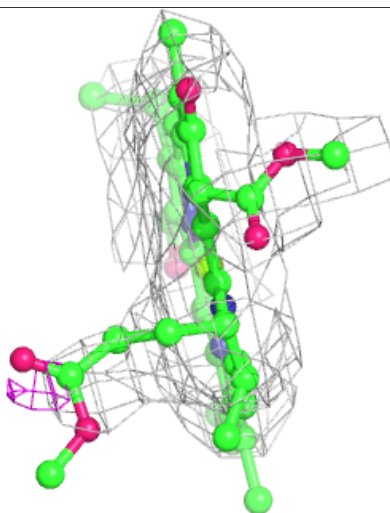
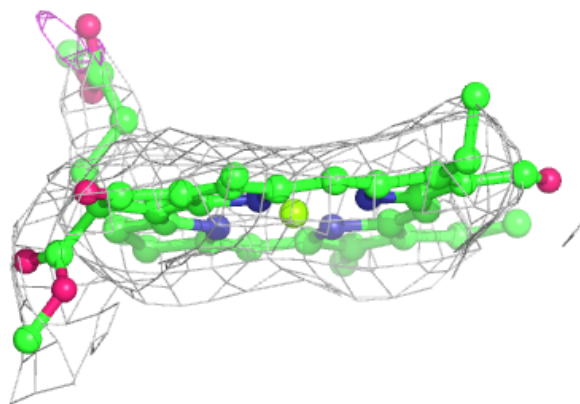
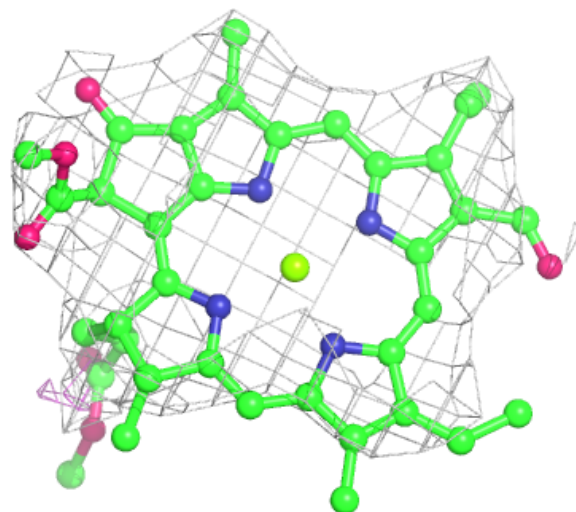
Electron density around LHG 1 801:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



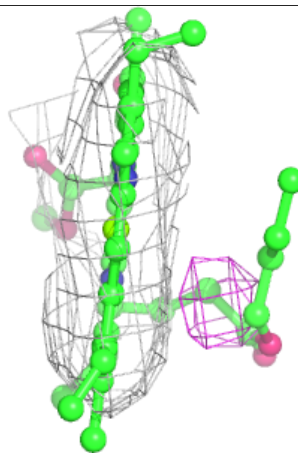
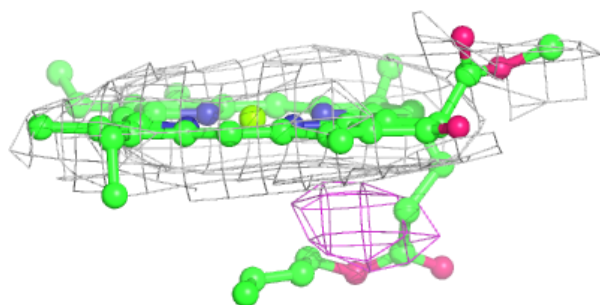
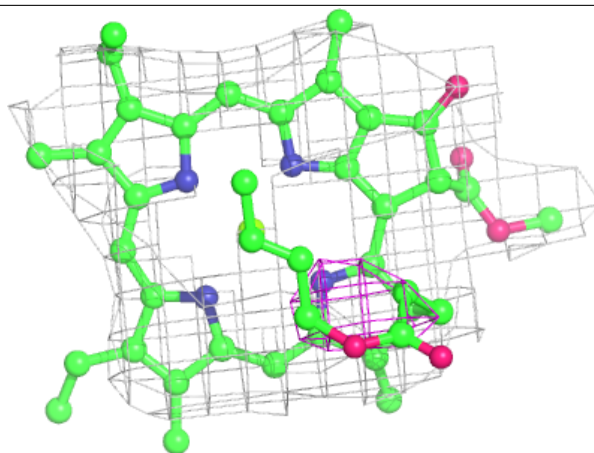
Electron density around CHL 4 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



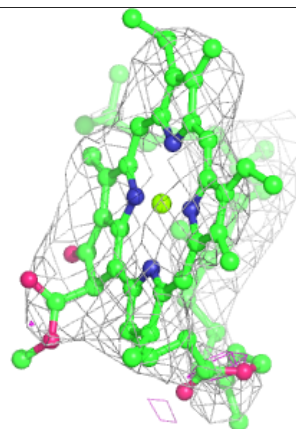
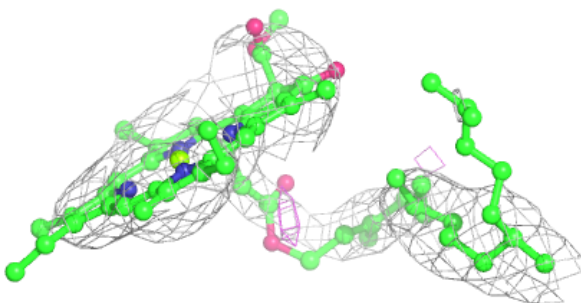
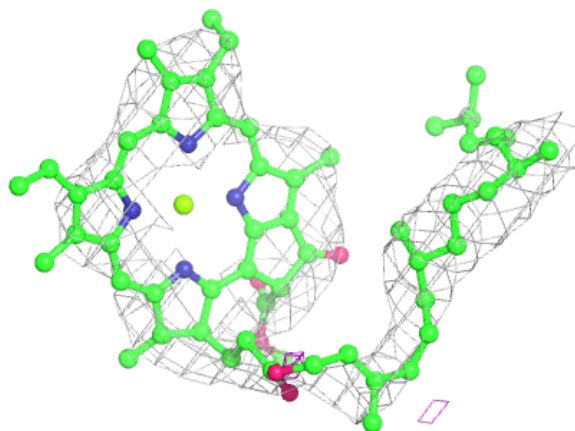
Electron density around CLA 2 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



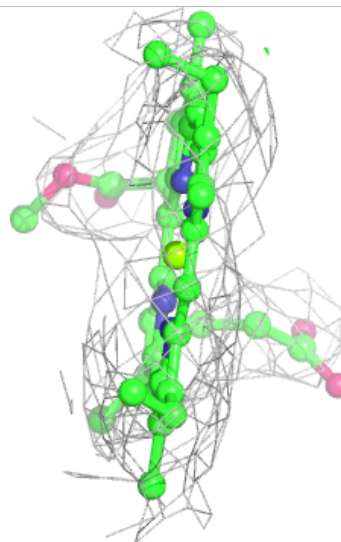
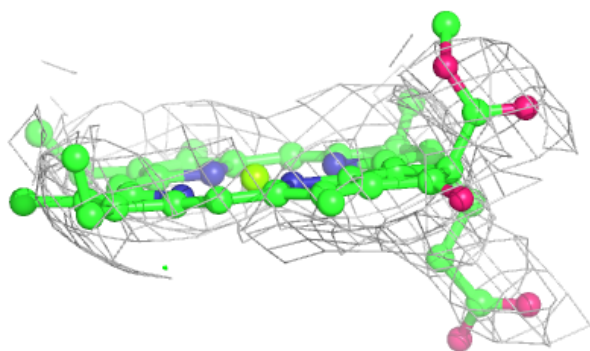
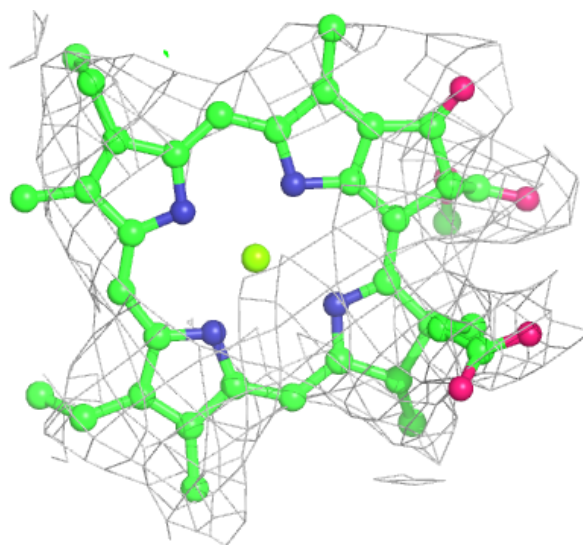
Electron density around CLA B 1229:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



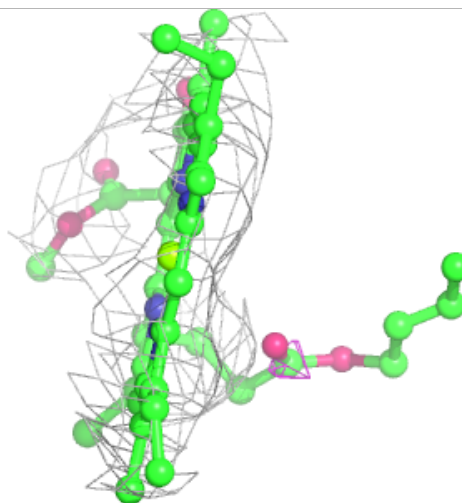
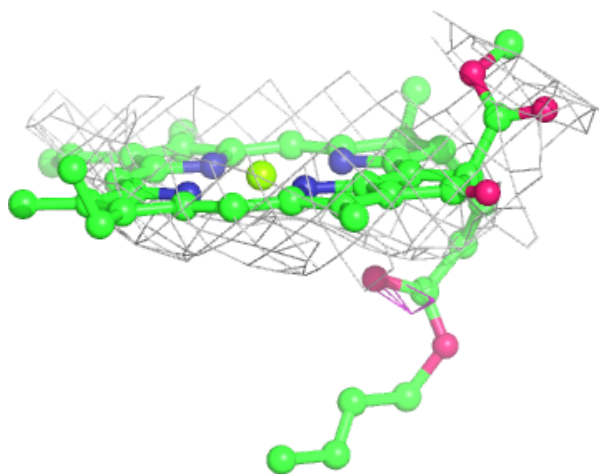
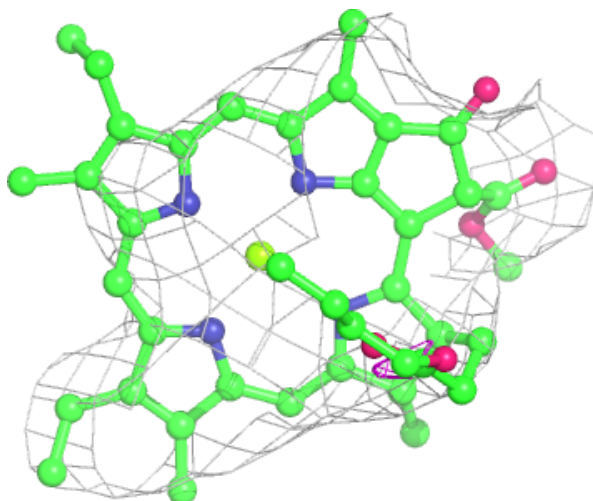
Electron density around CLA B 1227:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



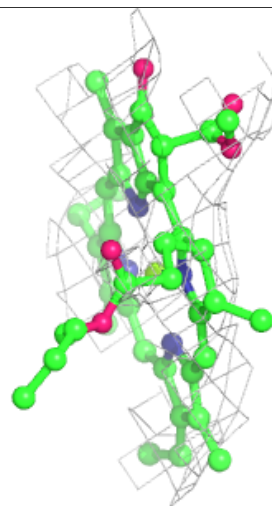
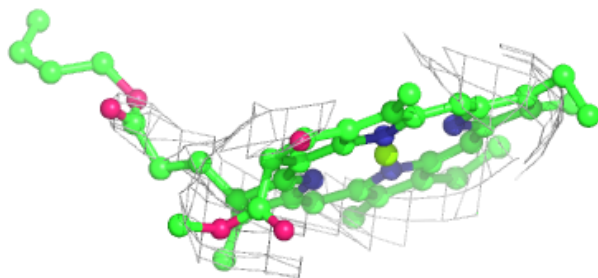
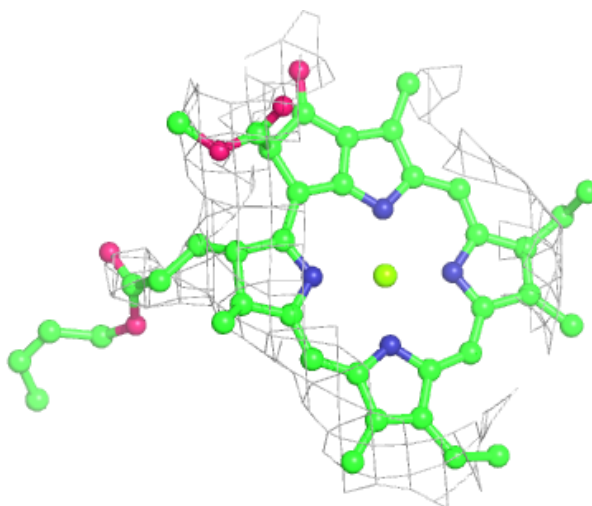
Electron density around CLA 2 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



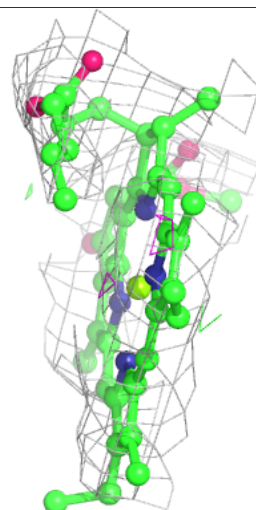
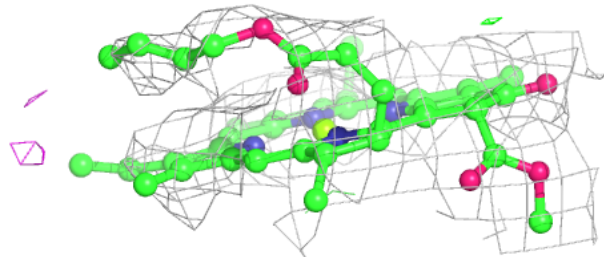
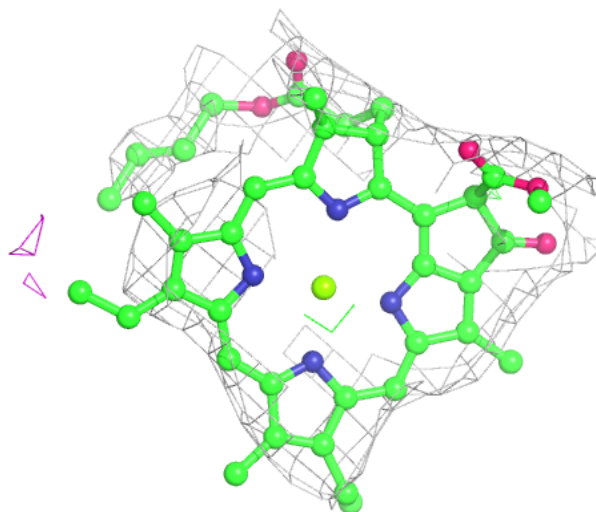
Electron density around CLA A 1125:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



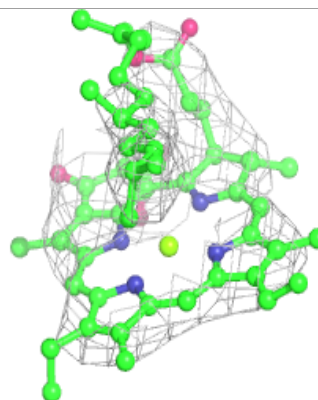
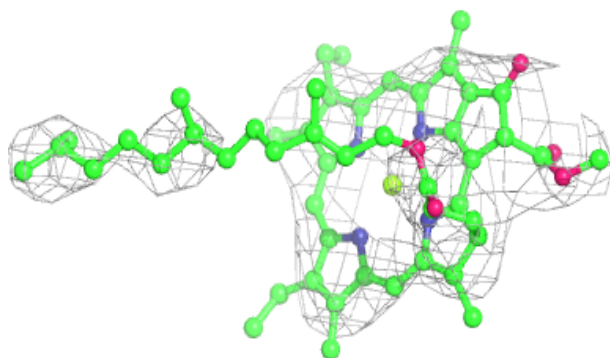
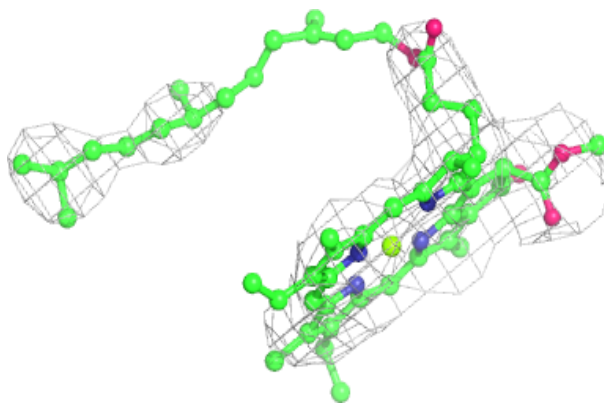
Electron density around CLA 1 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

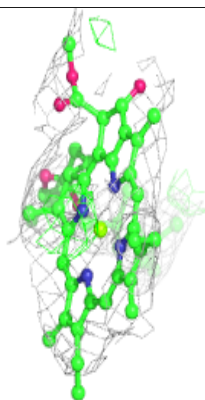
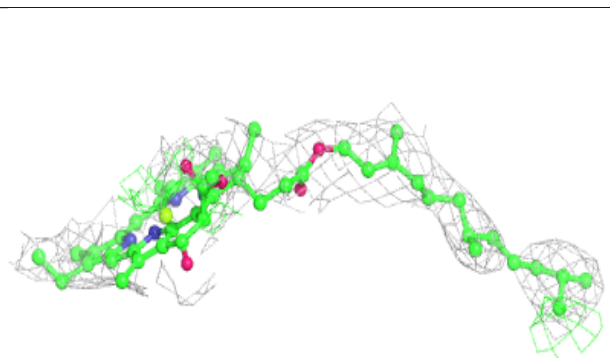
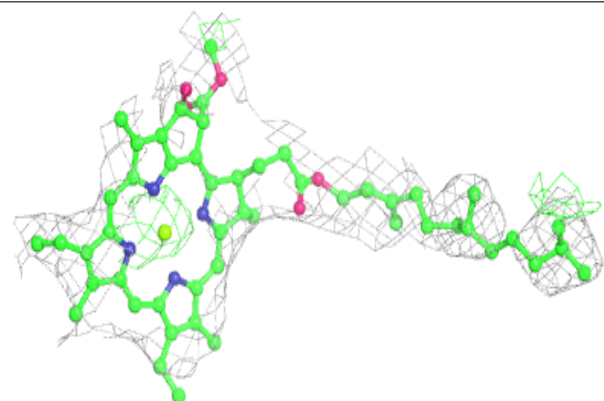


Electron density around CLA B 1228:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

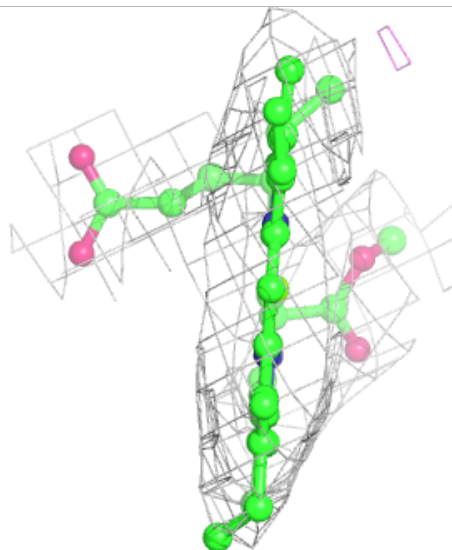
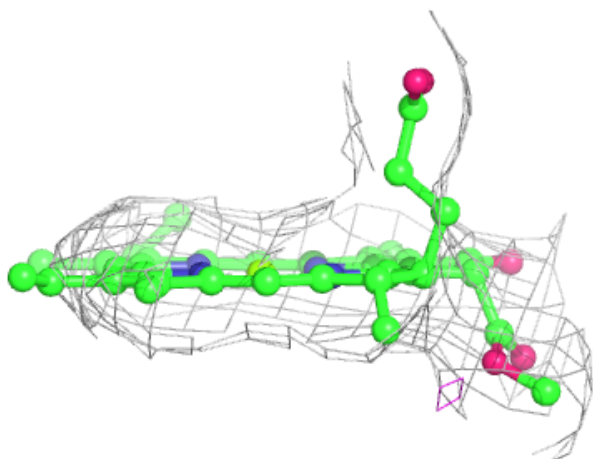
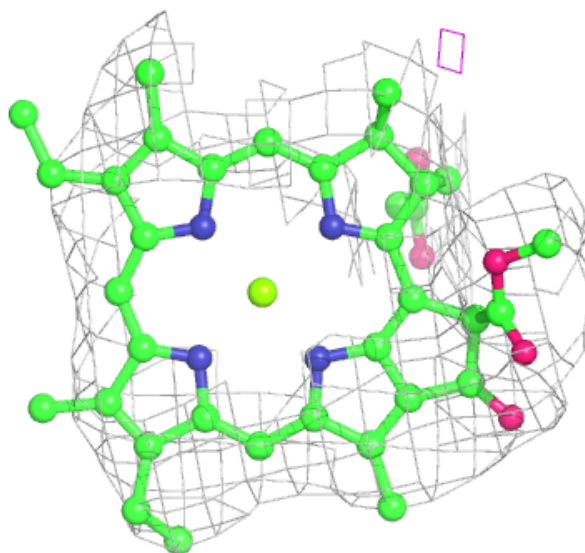
**Electron density around CLA A 1012:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



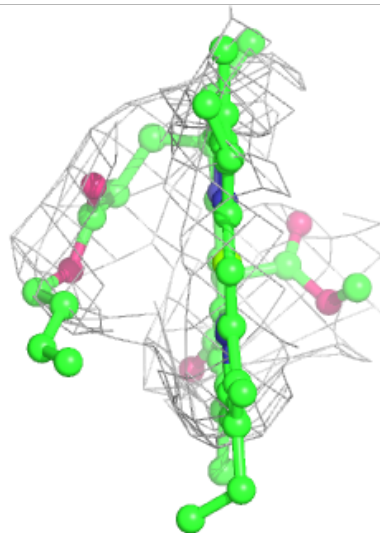
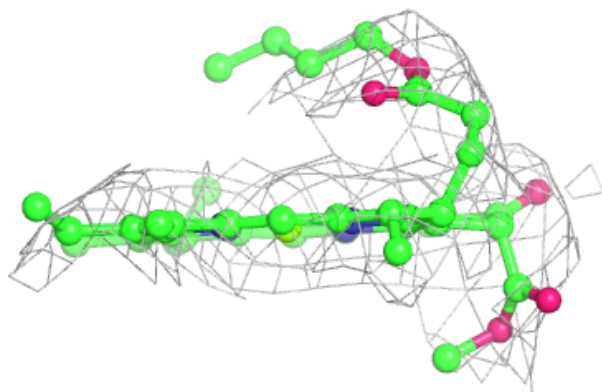
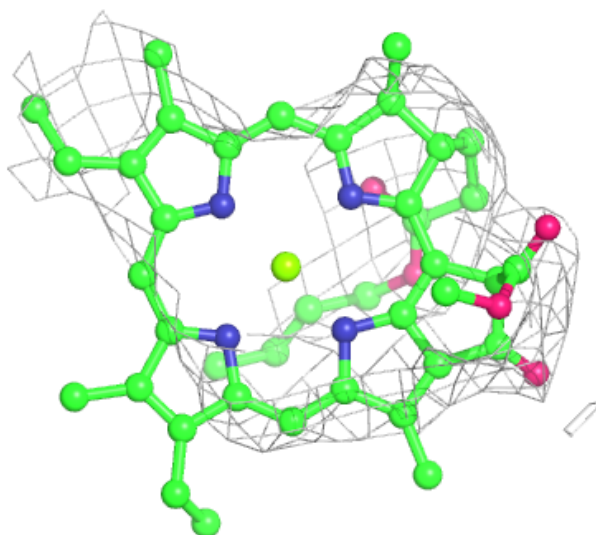
Electron density around CLA 1 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



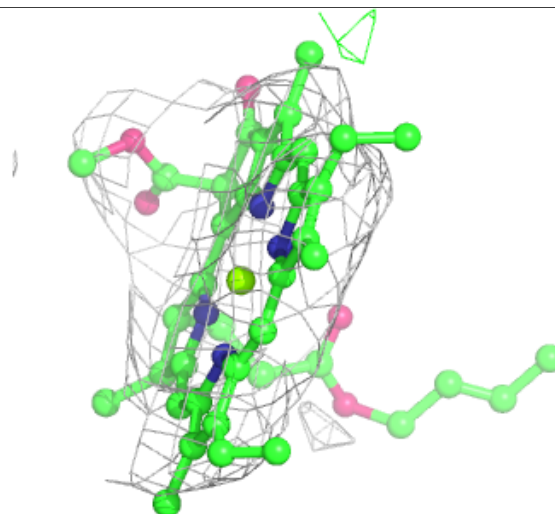
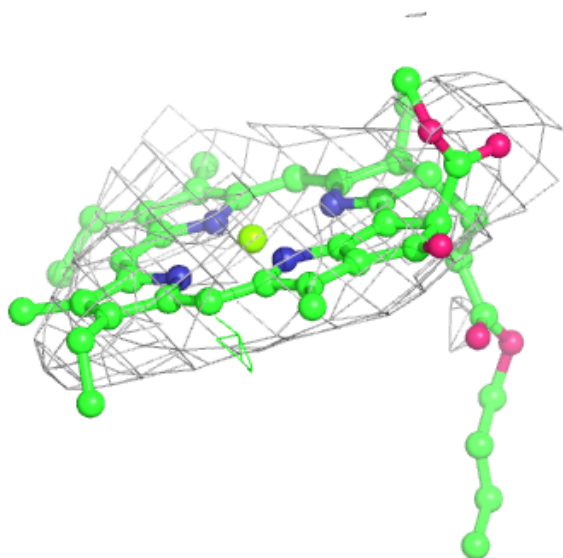
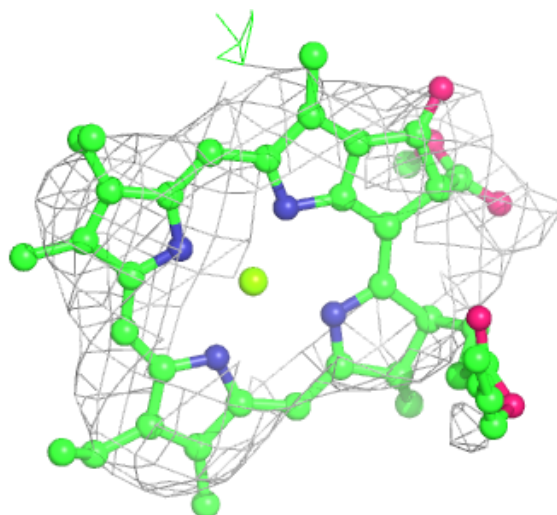
Electron density around CLA A 1110:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



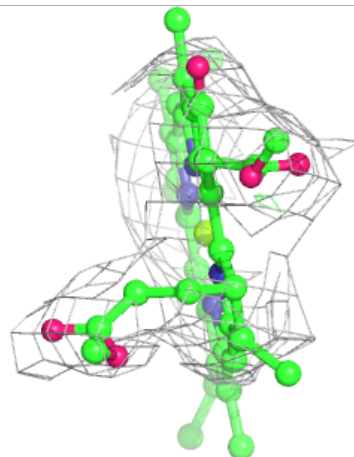
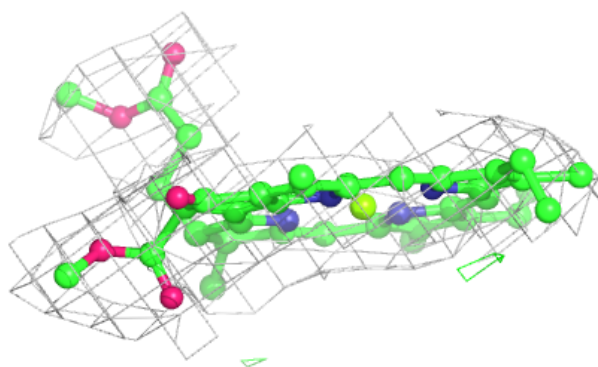
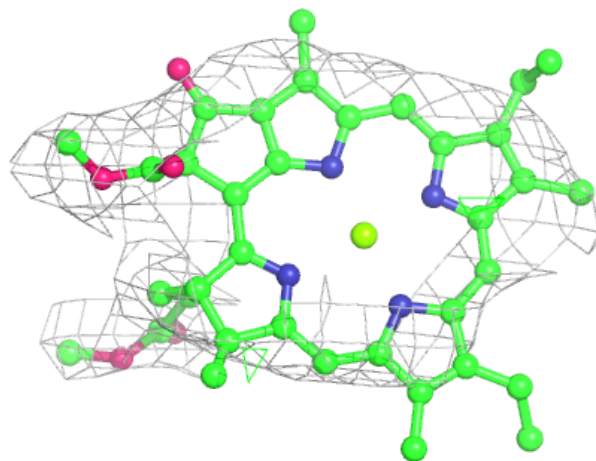
Electron density around CLA A 1122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



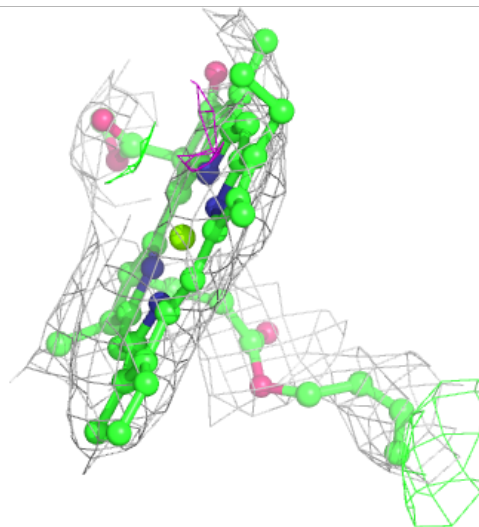
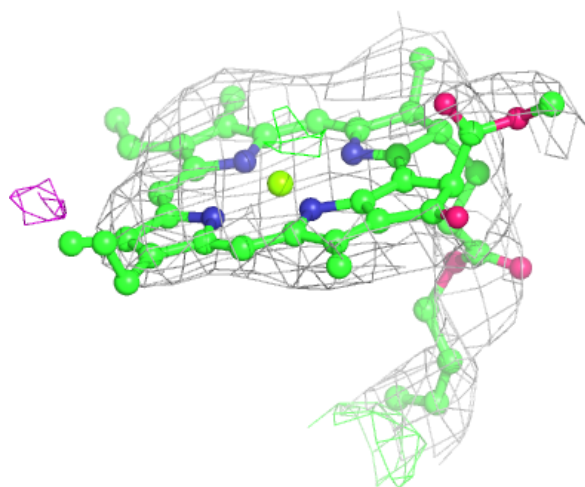
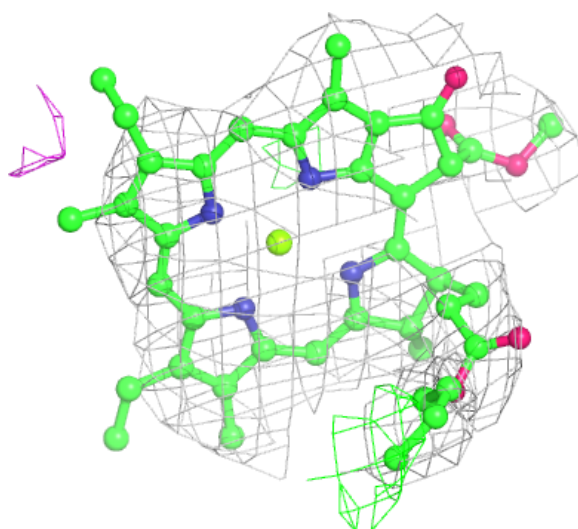
Electron density around CLA 3 615:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



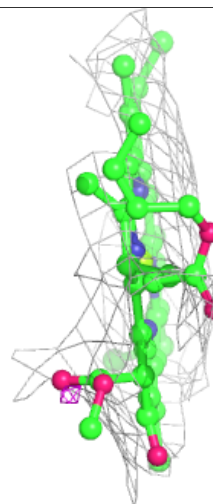
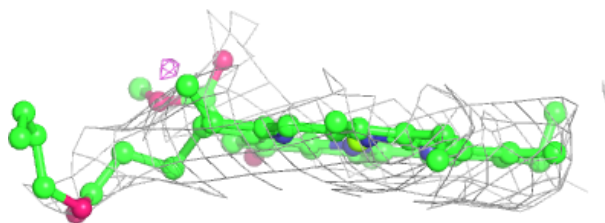
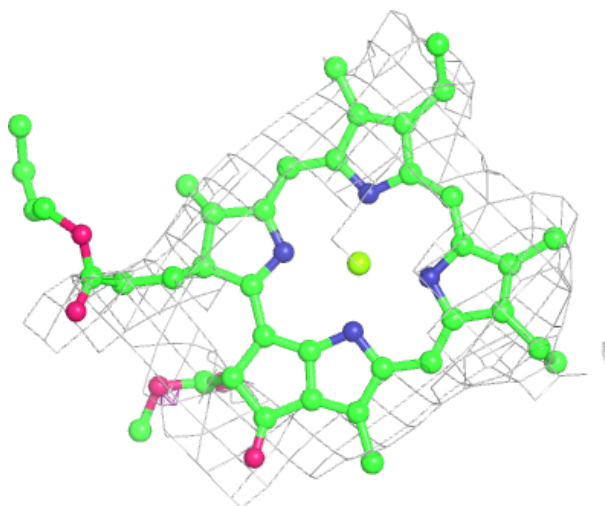
Electron density around CLA B 1216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



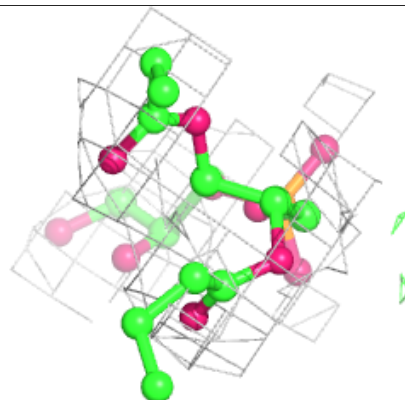
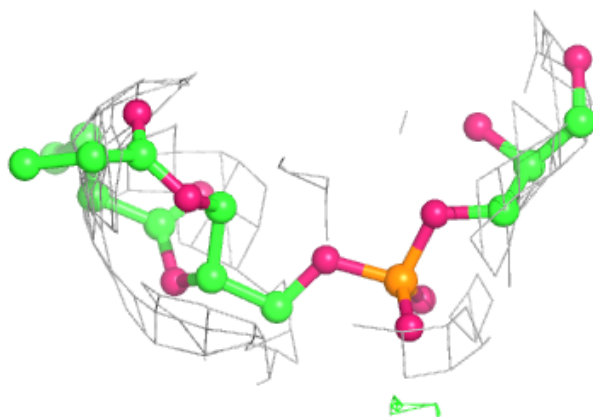
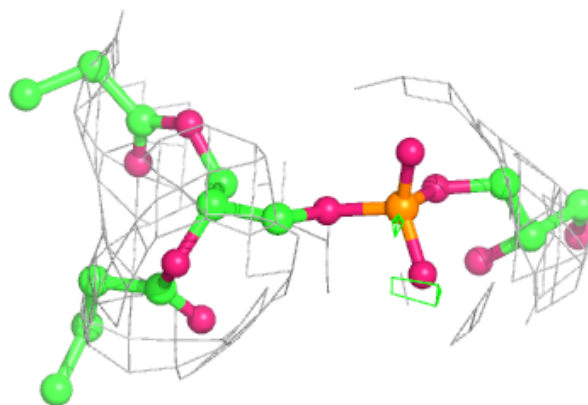
Electron density around CLA B 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



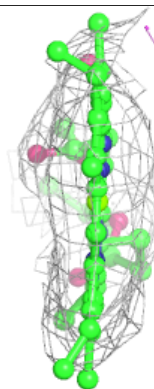
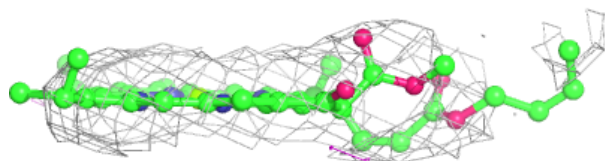
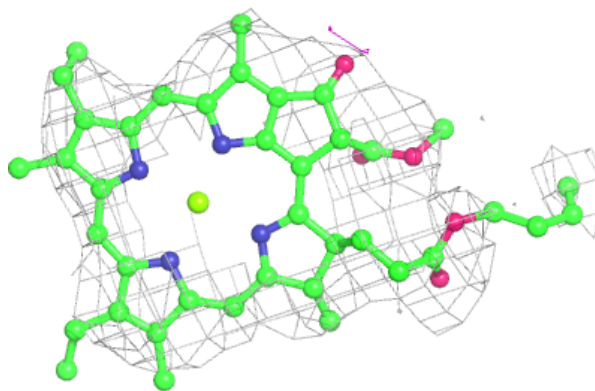
Electron density around LHG A 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



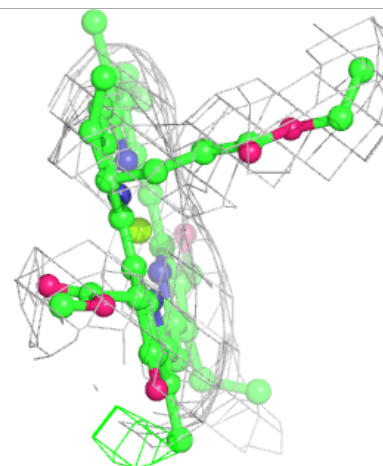
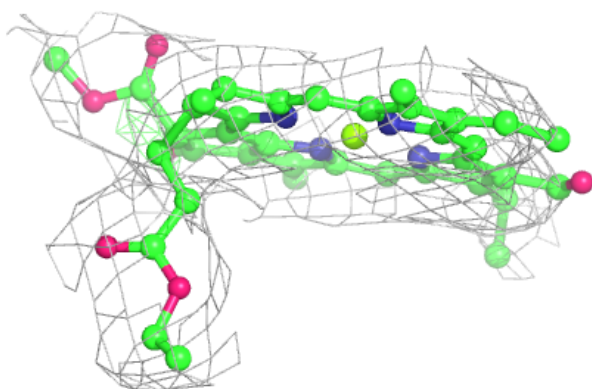
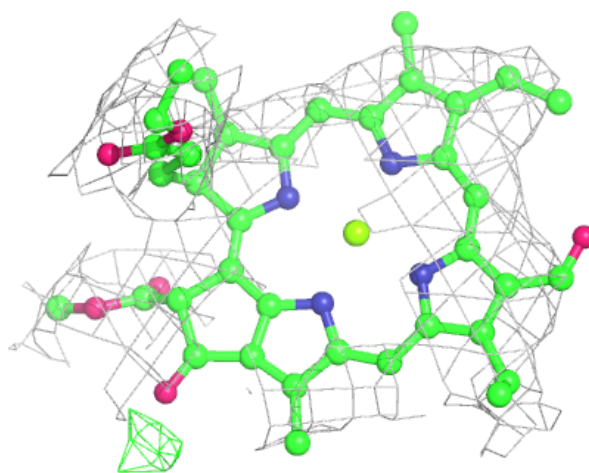
Electron density around CLA 4 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



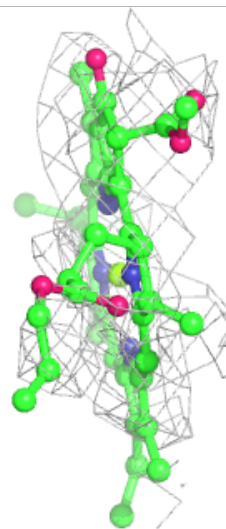
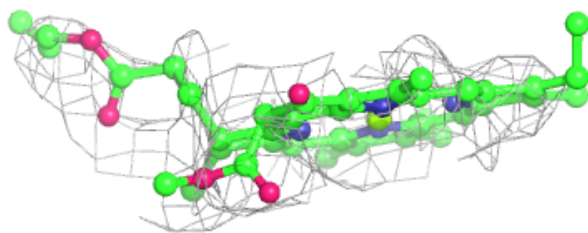
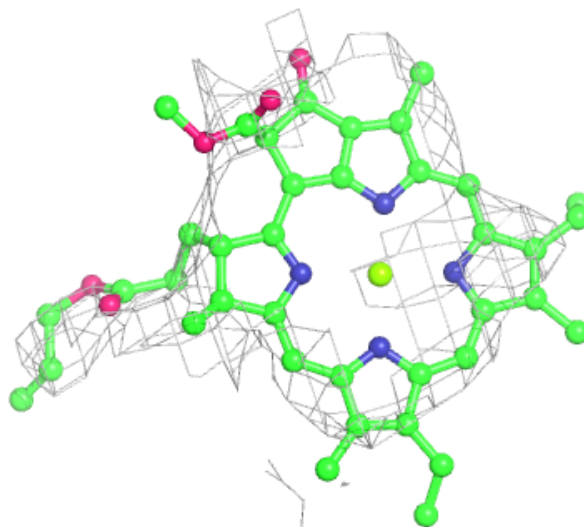
Electron density around CHL 2 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



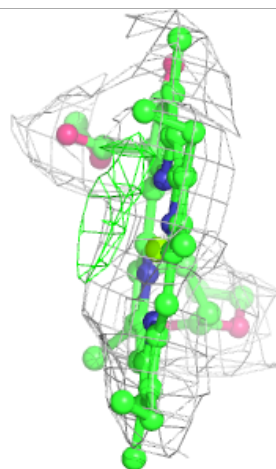
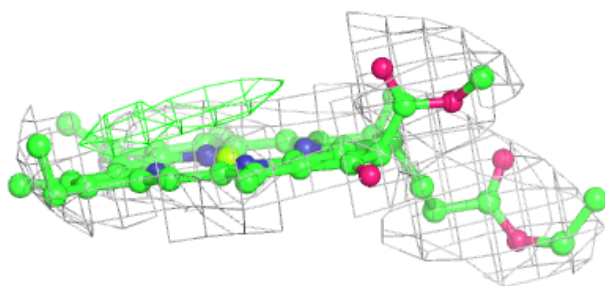
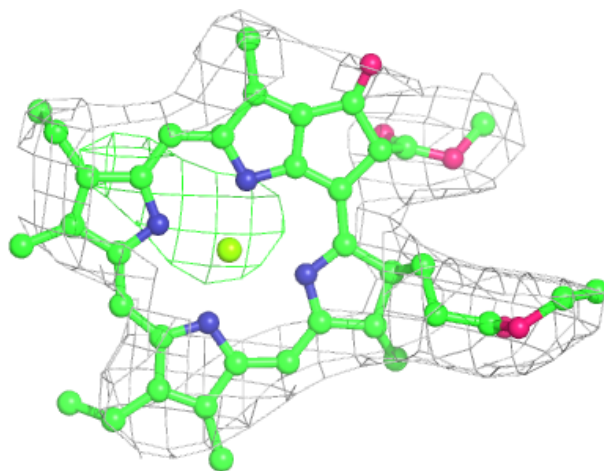
Electron density around CLA A 1129:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



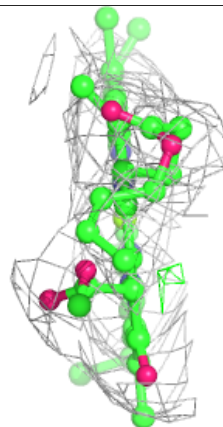
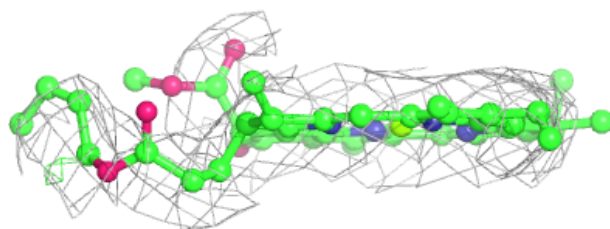
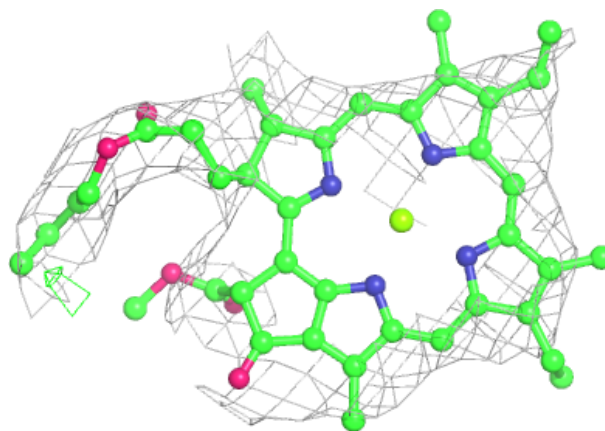
Electron density around CLA F 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



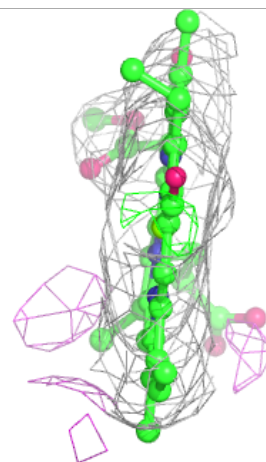
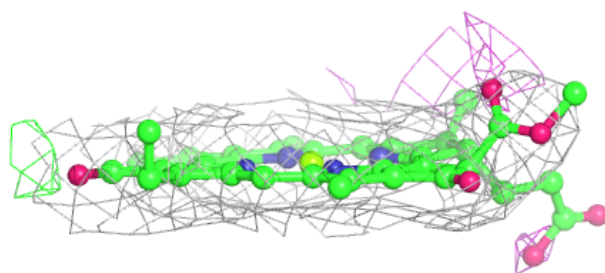
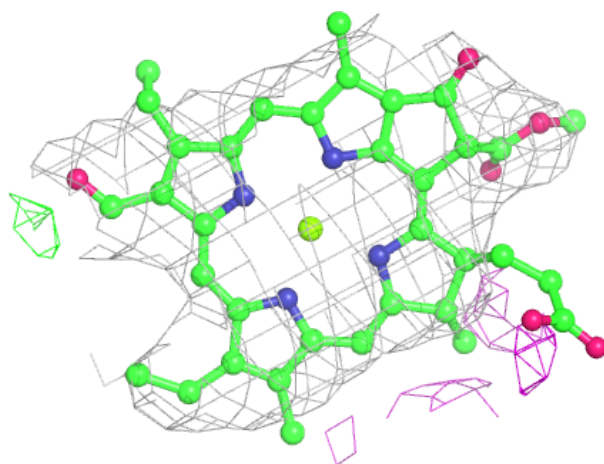
Electron density around CLA B 1202:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



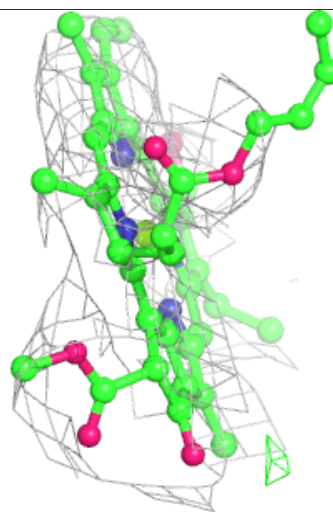
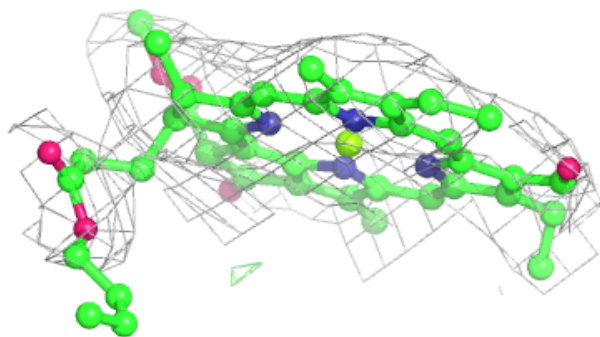
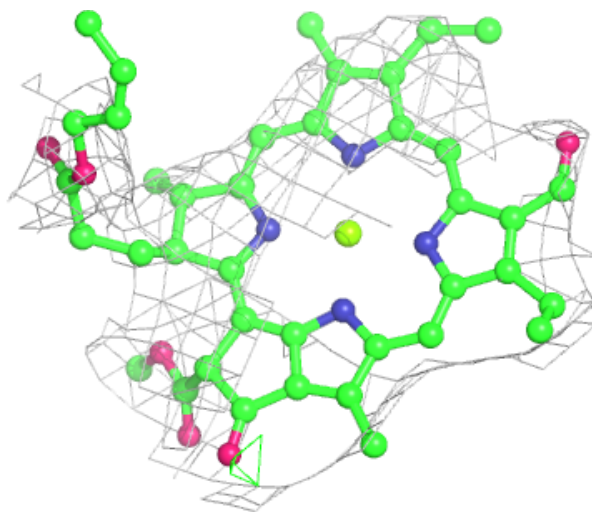
Electron density around CHL 2 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



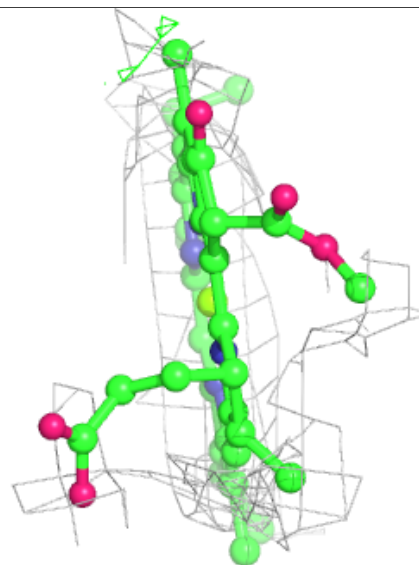
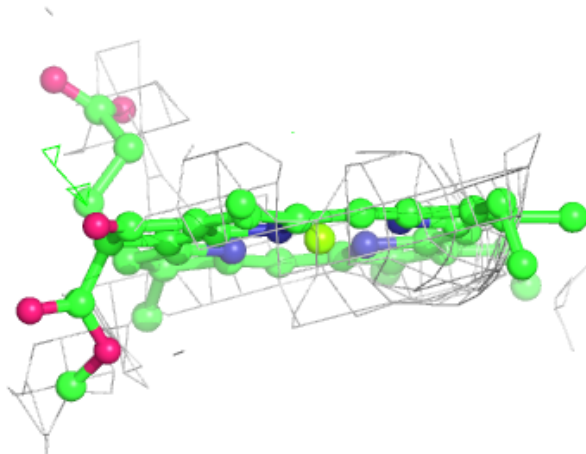
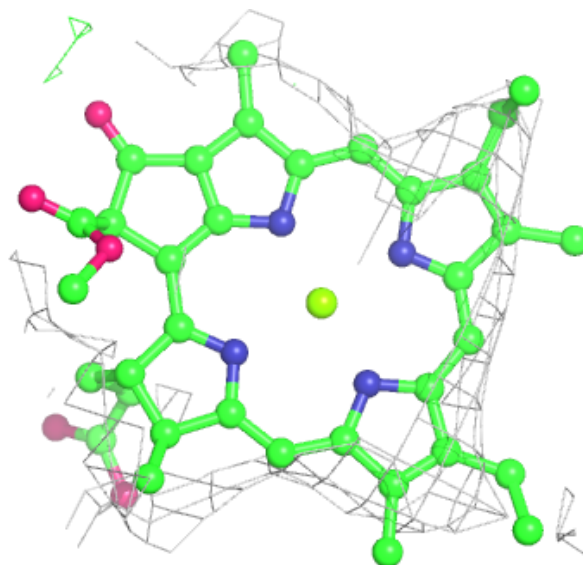
Electron density around CHL 2 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



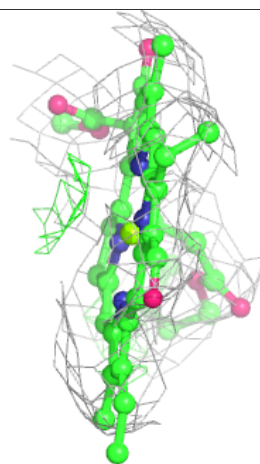
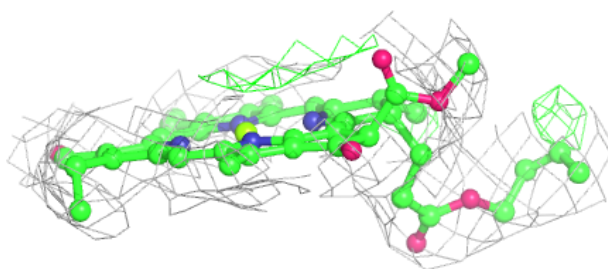
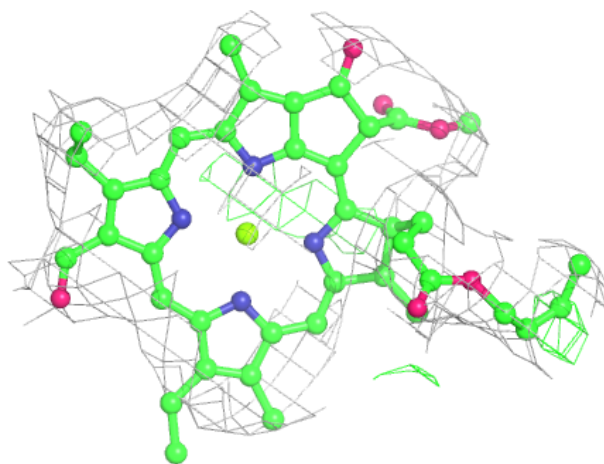
Electron density around CLA A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



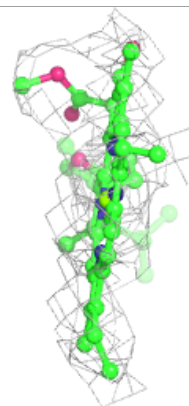
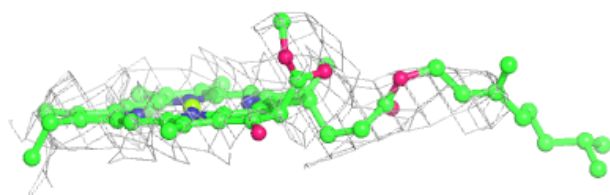
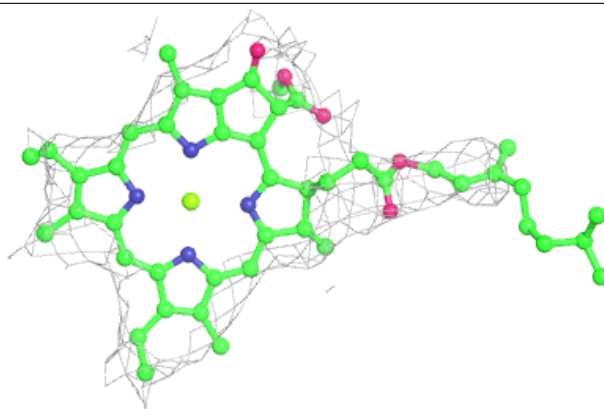
Electron density around CHL 2 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



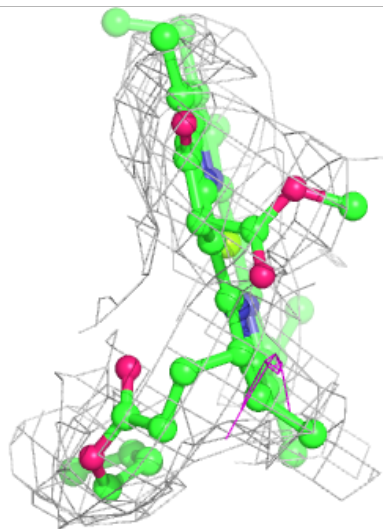
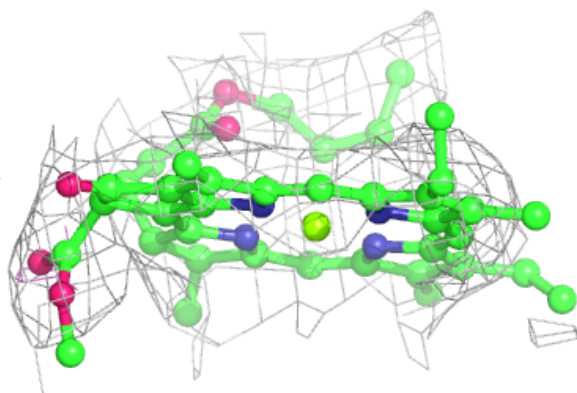
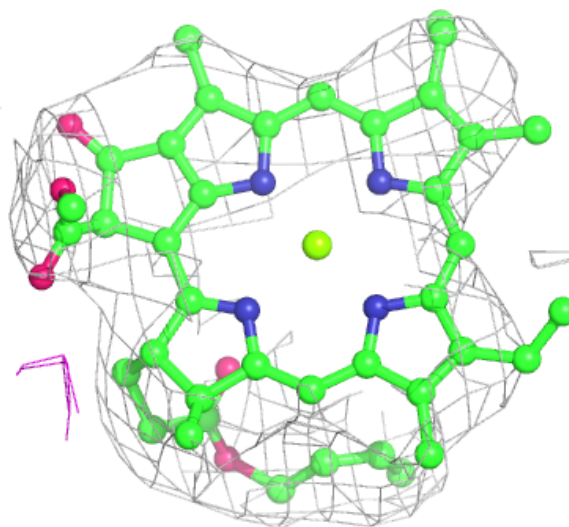
Electron density around CLA A 1103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



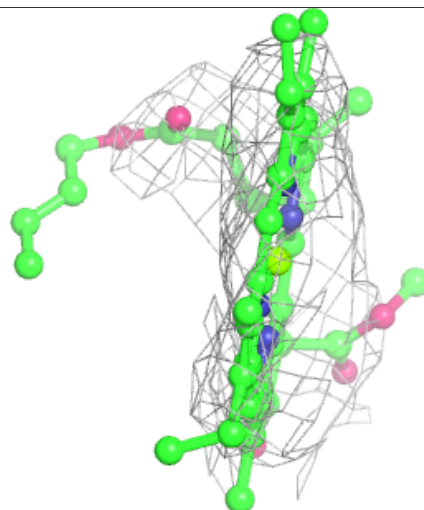
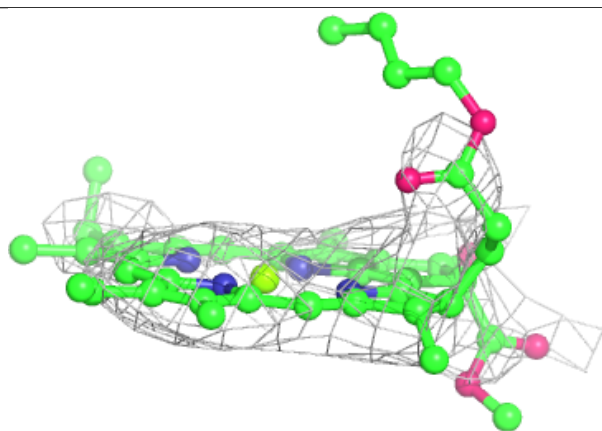
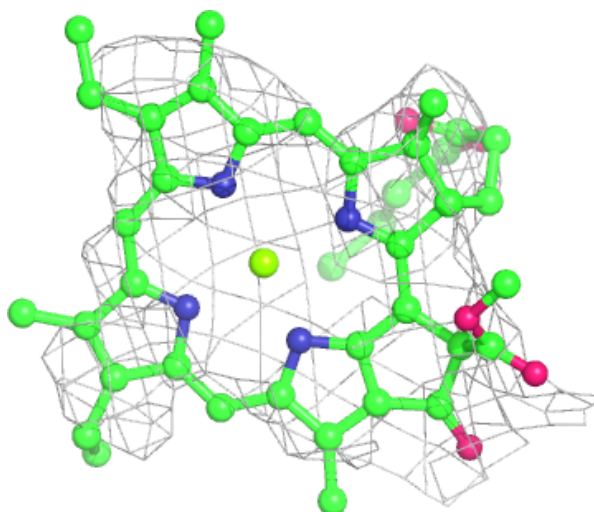
Electron density around CLA 4 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



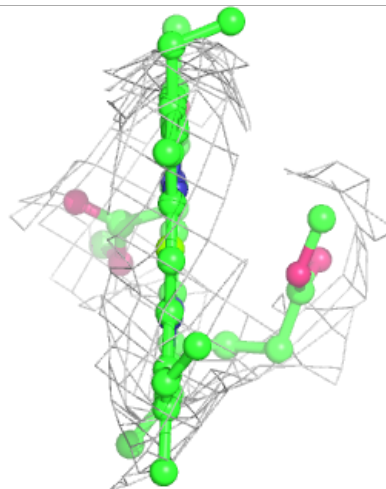
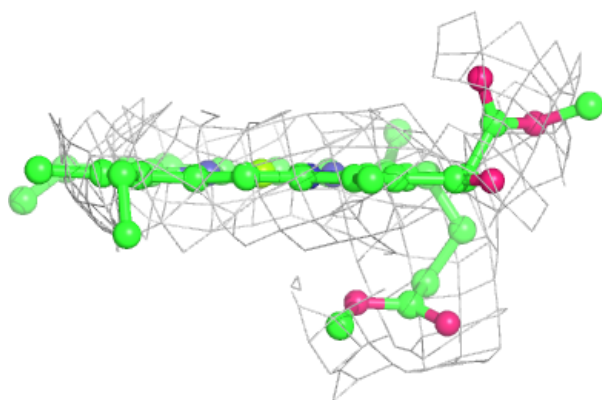
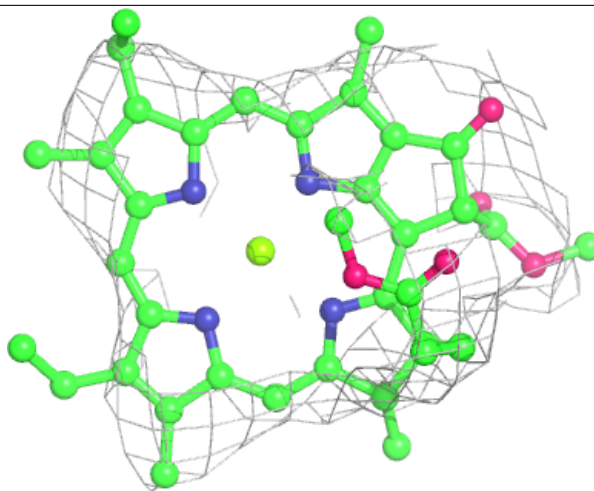
Electron density around CLA A 1115:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



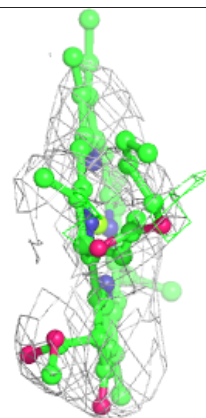
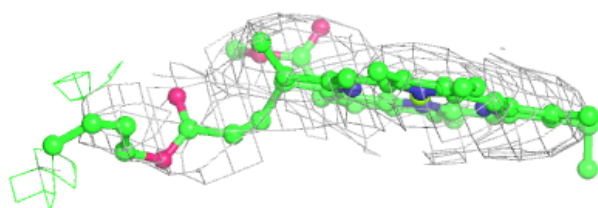
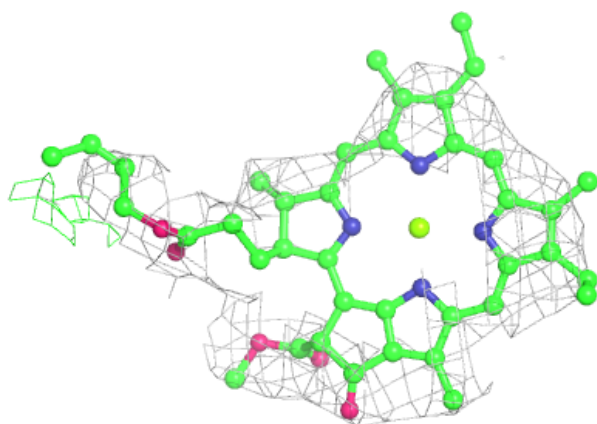
Electron density around CLA 2 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

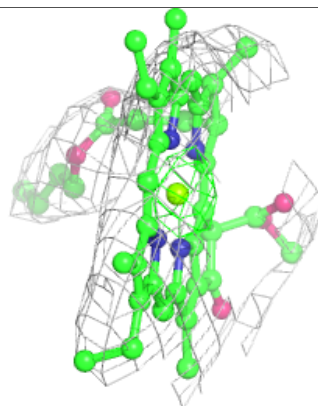
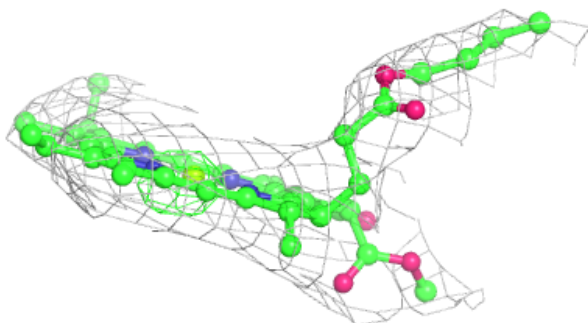
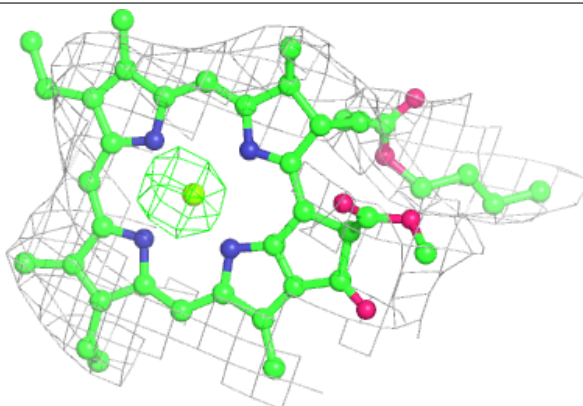


Electron density around CLA J 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

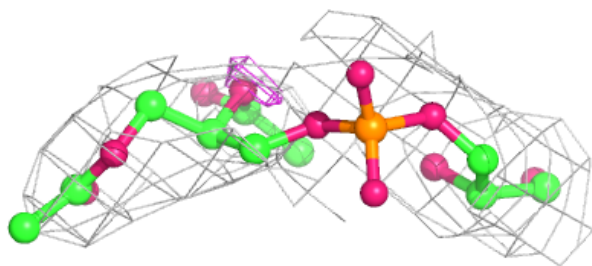
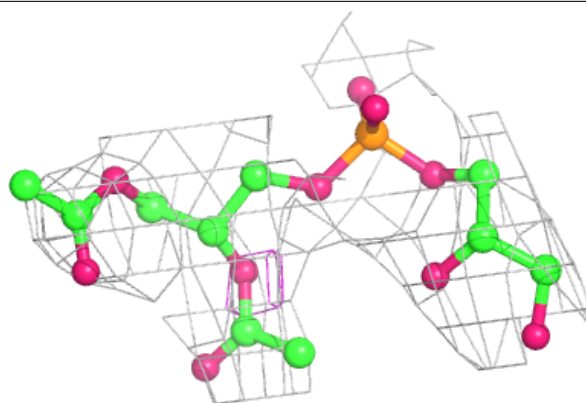
**Electron density around CLA A 1107:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

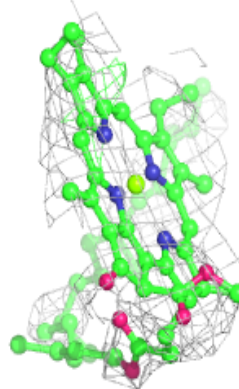
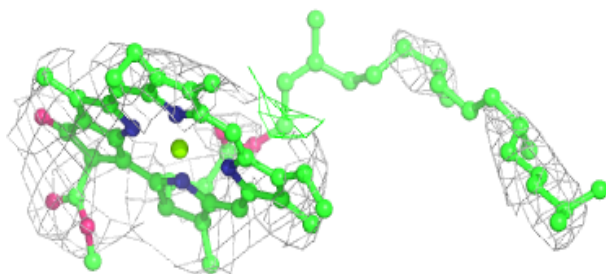
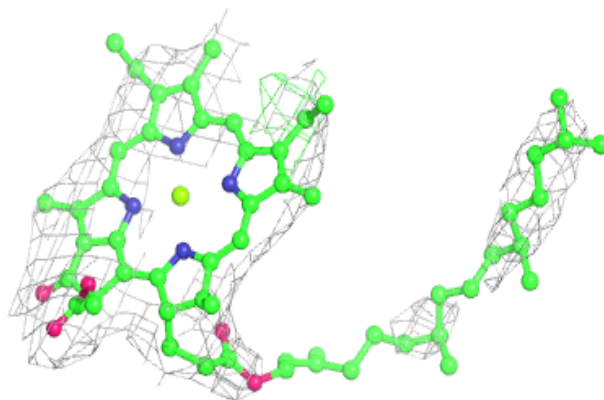


Electron density around LHG B 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

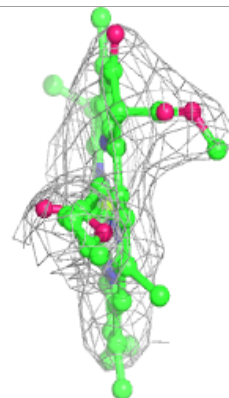
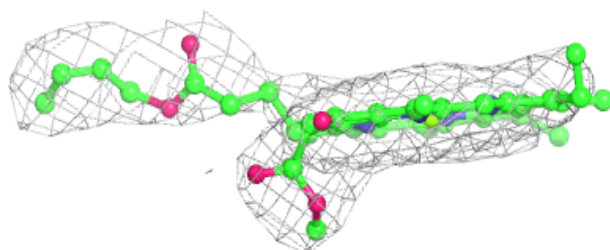
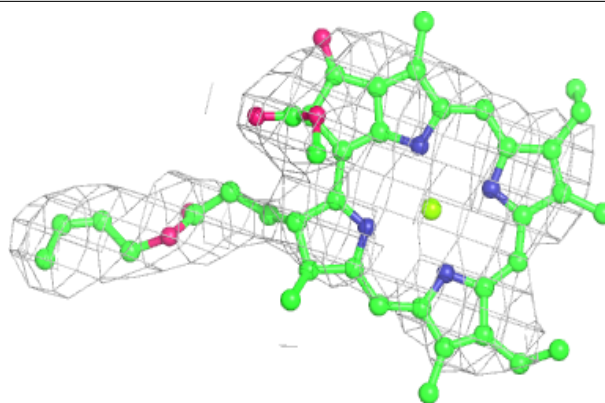
**Electron density around CLA A 1106:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

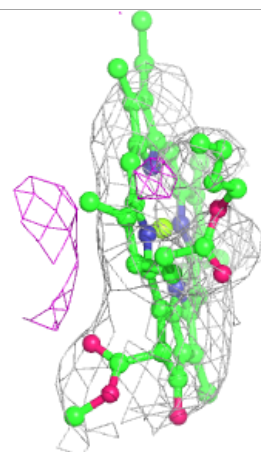
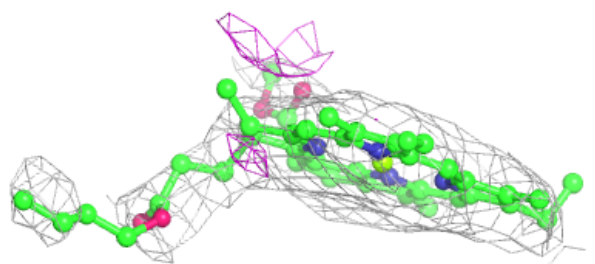
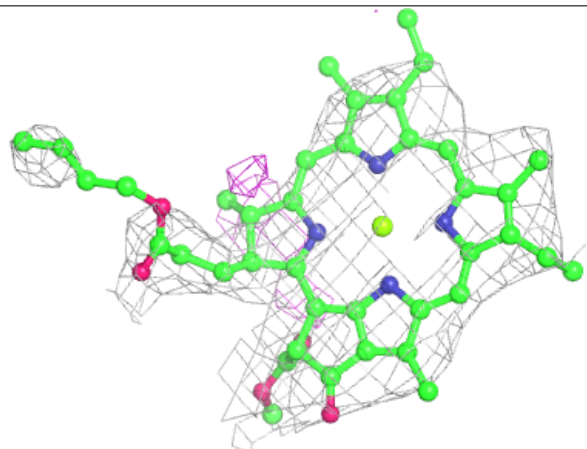


Electron density around CLA B 1234:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

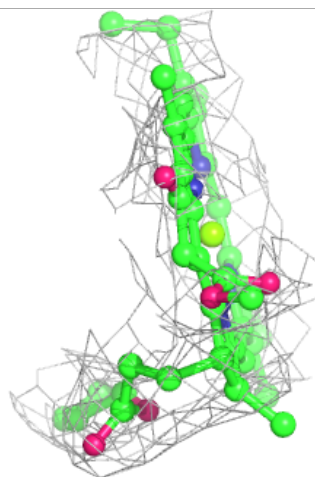
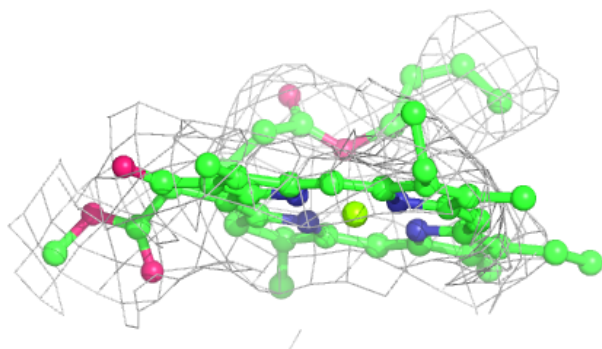
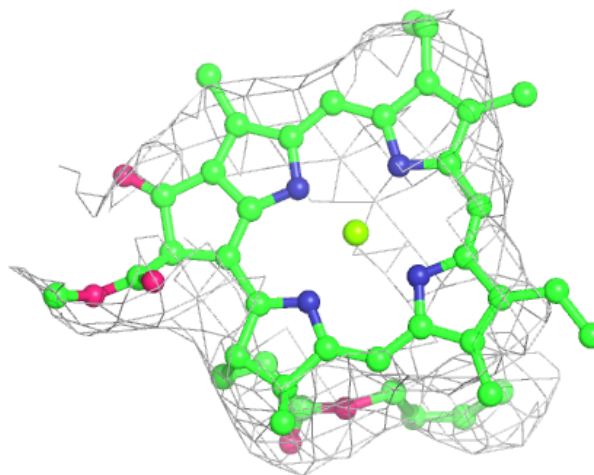
**Electron density around CLA 4 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



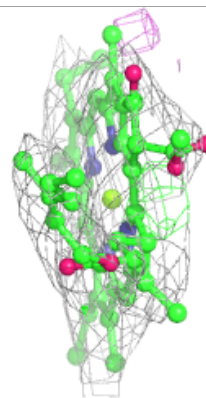
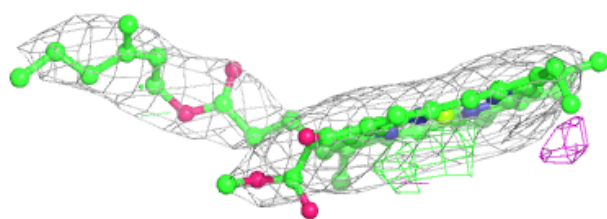
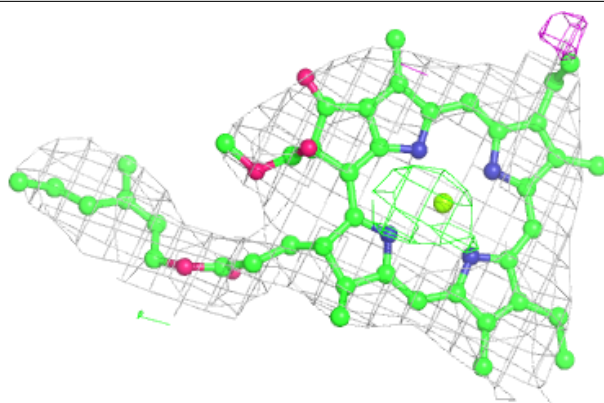
Electron density around CLA 4 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



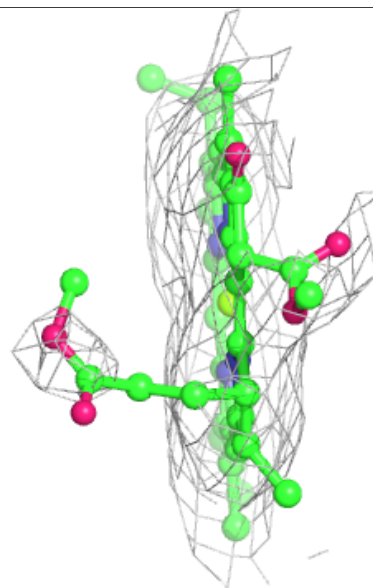
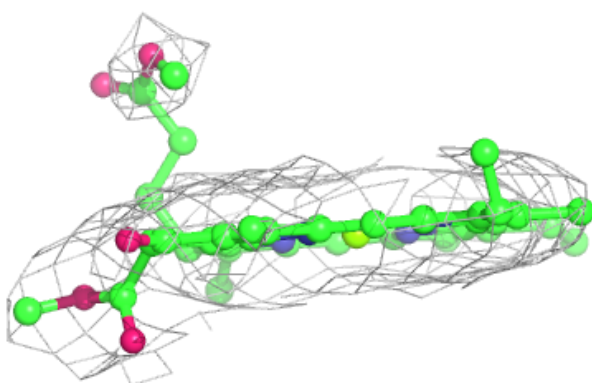
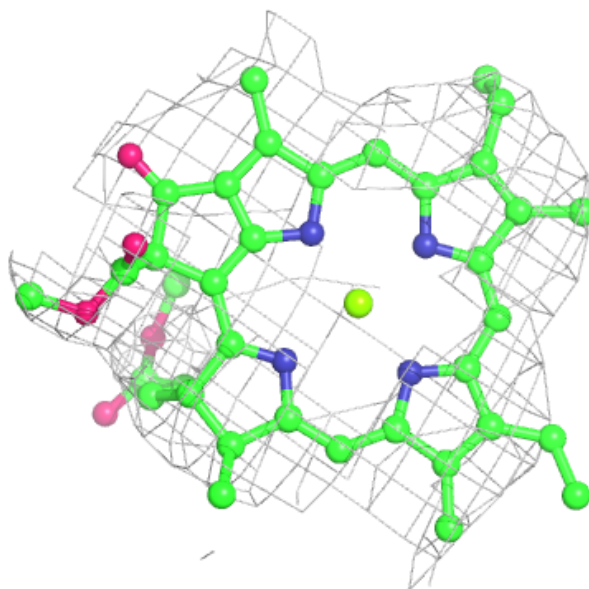
Electron density around CLA A 1139:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



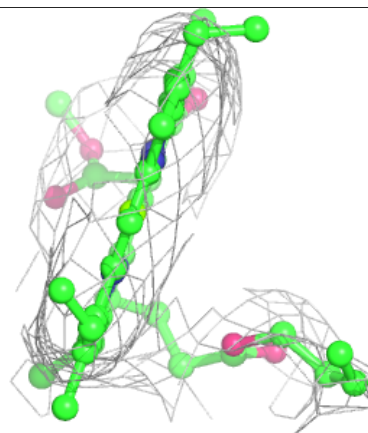
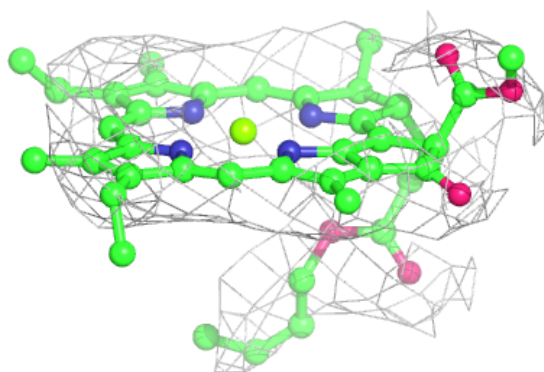
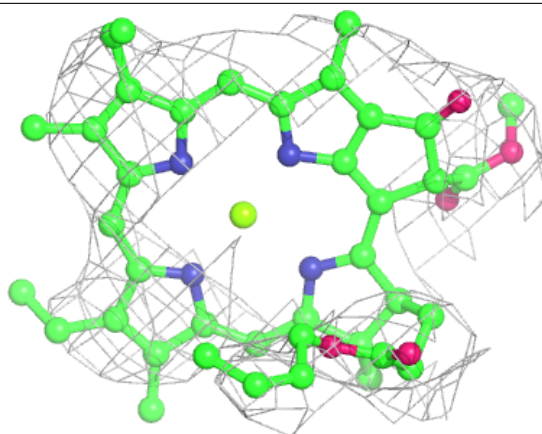
Electron density around CLA 4 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



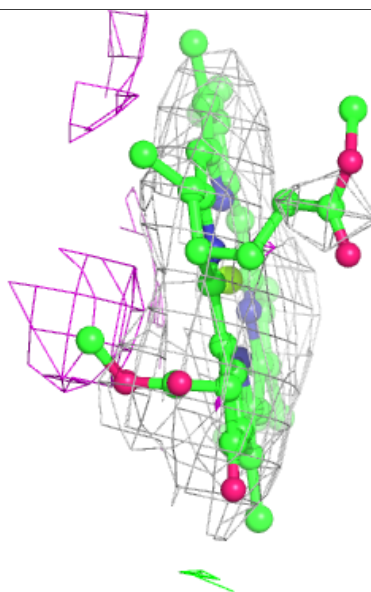
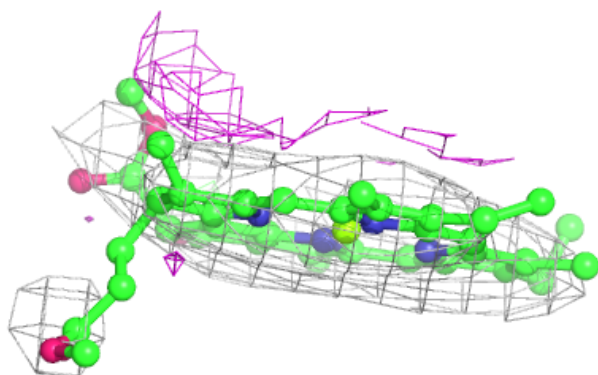
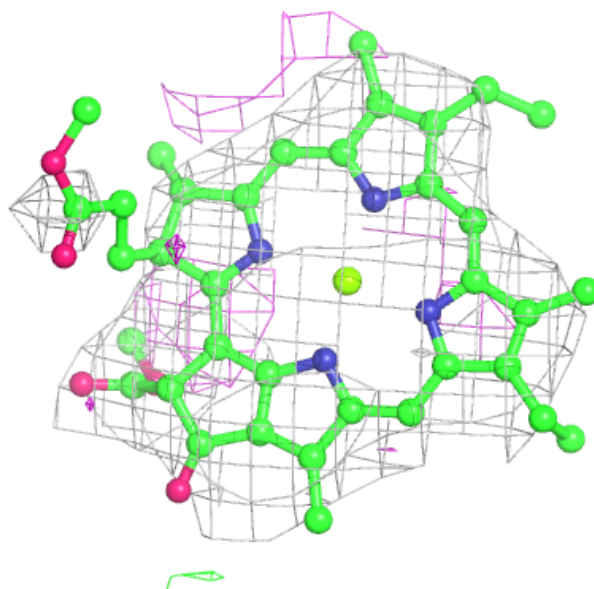
Electron density around CLA A 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



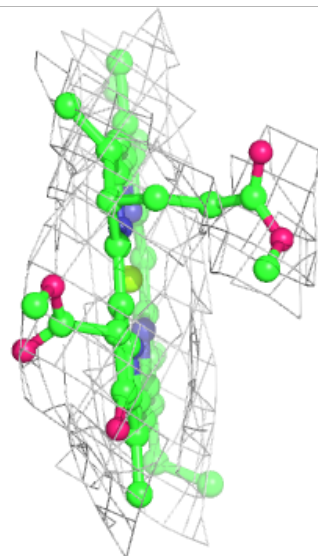
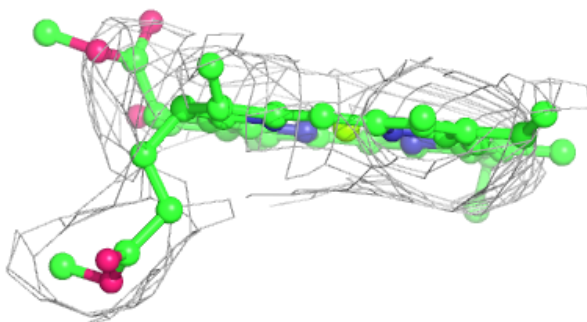
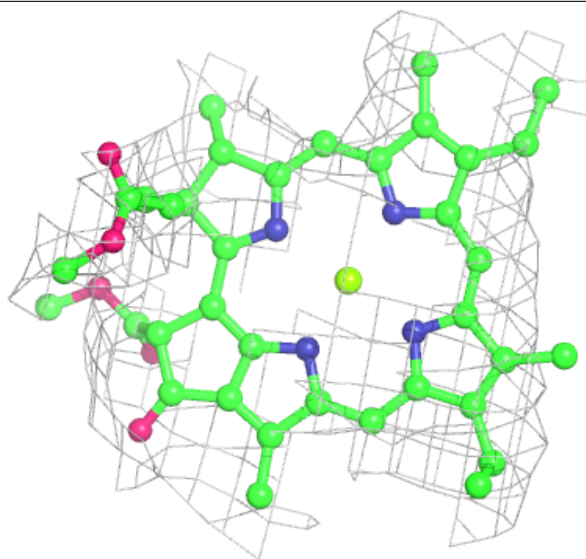
Electron density around CLA 1 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



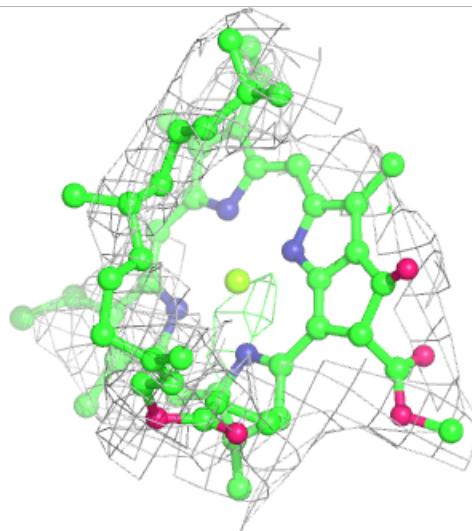
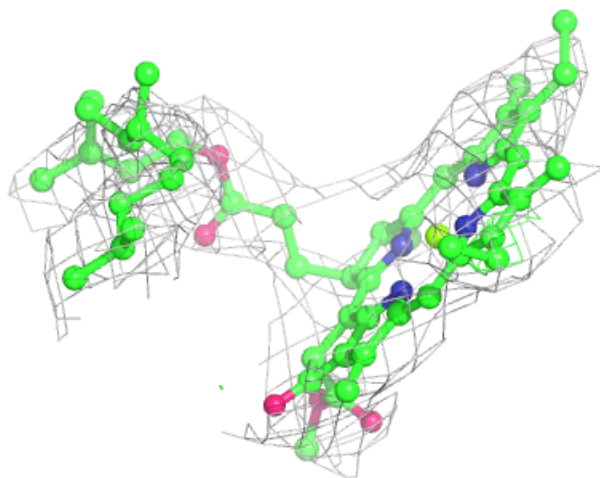
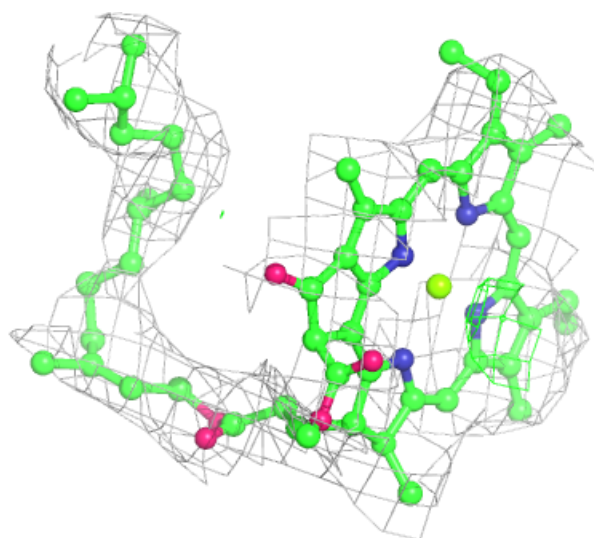
Electron density around CLA B 1209:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



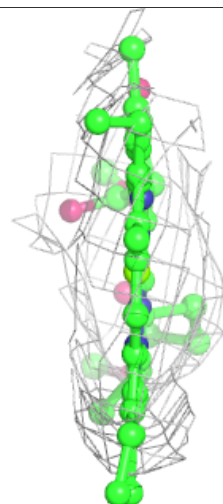
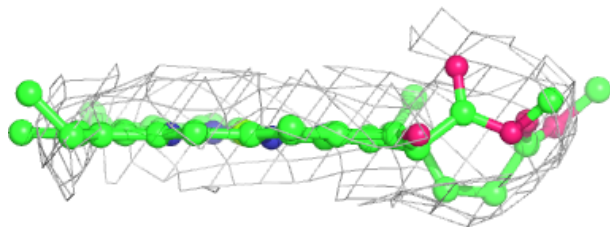
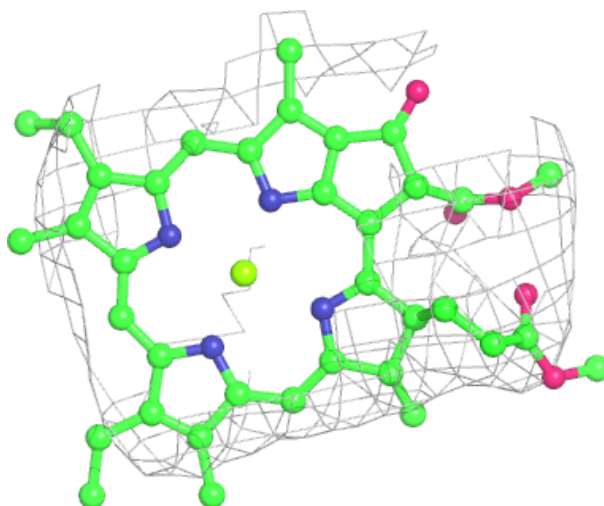
Electron density around CLA B 1231:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



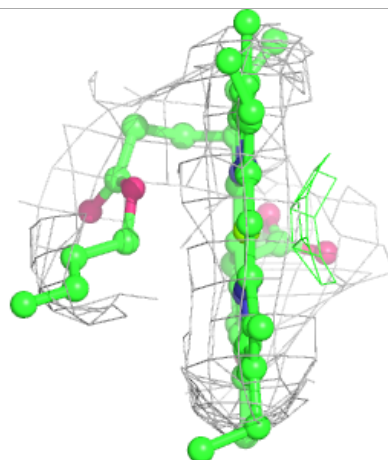
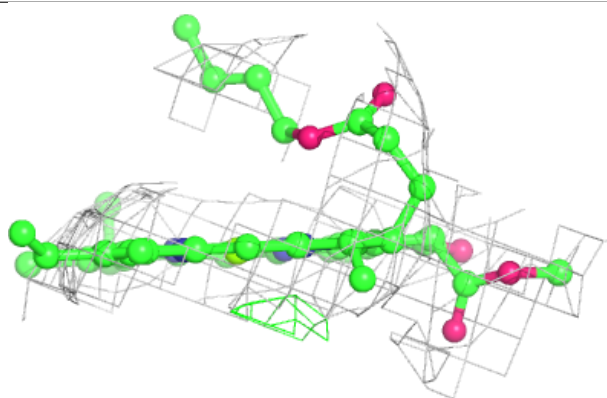
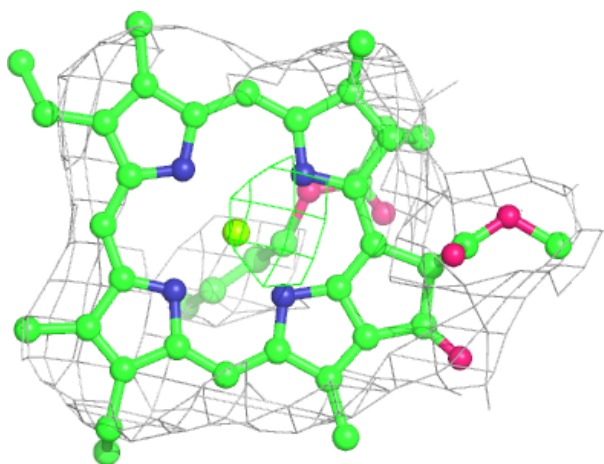
Electron density around CLA 3 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



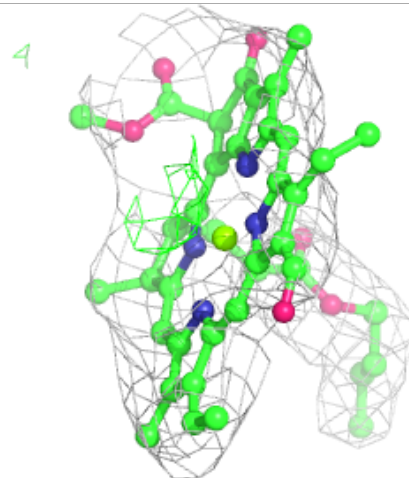
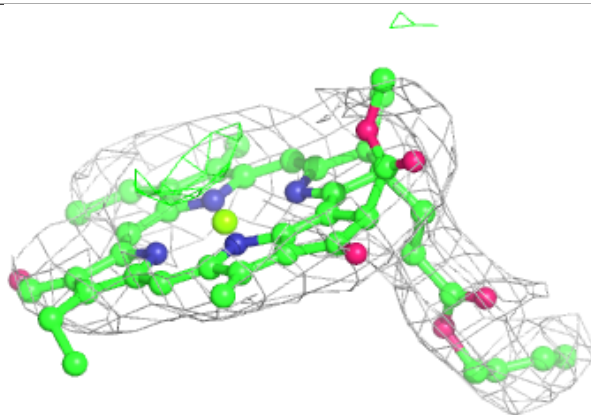
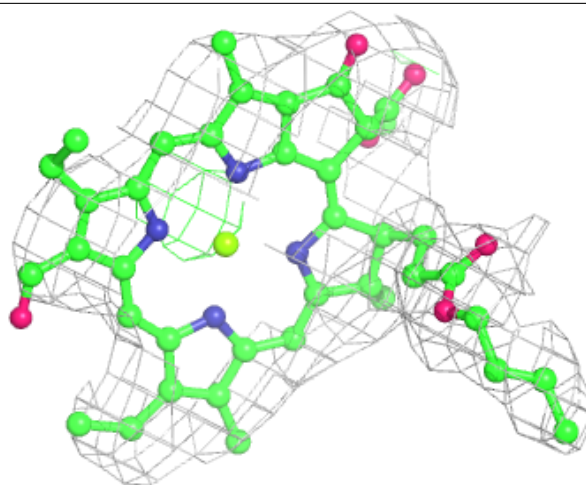
Electron density around CLA 4 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



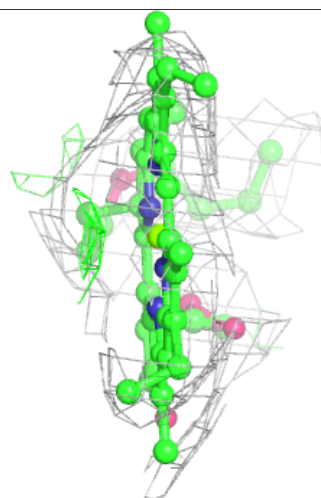
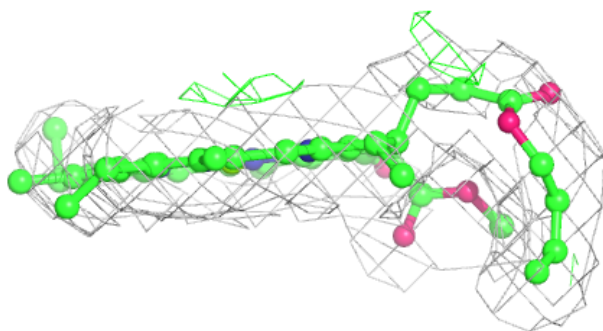
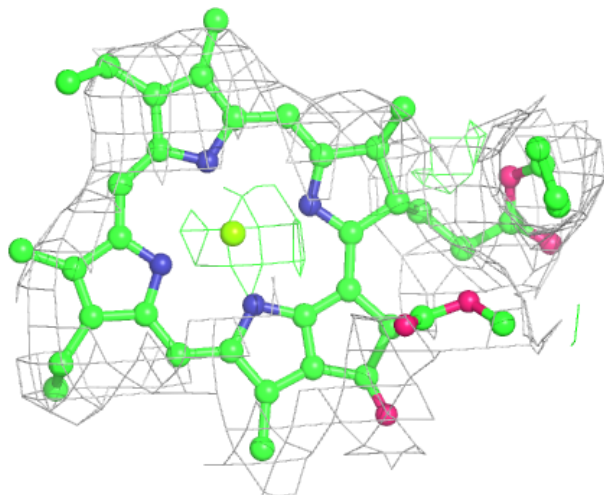
Electron density around CHL 4 611:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



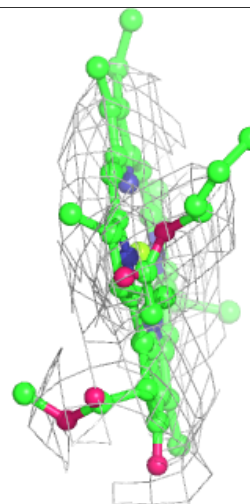
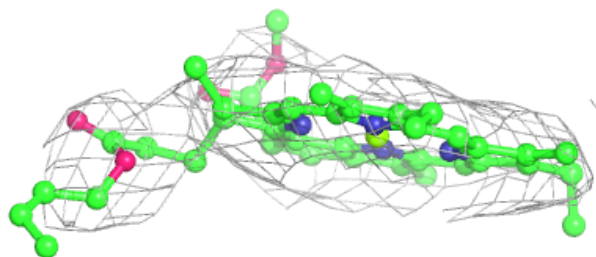
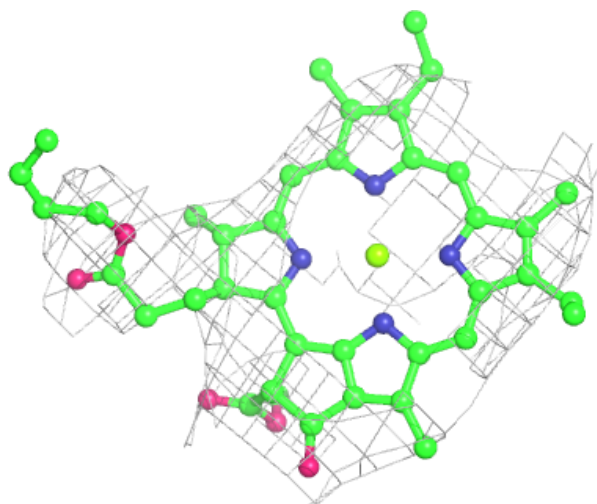
Electron density around CLA 4 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



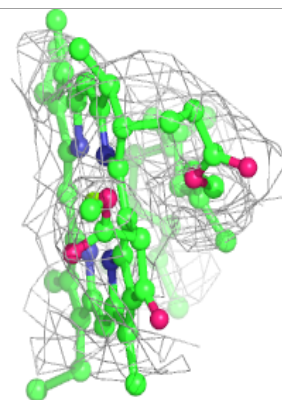
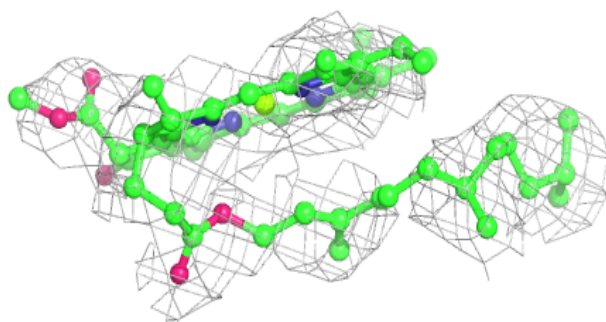
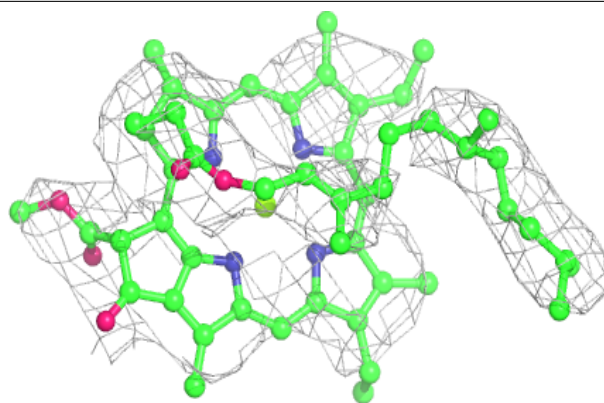
Electron density around CLA B 1210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



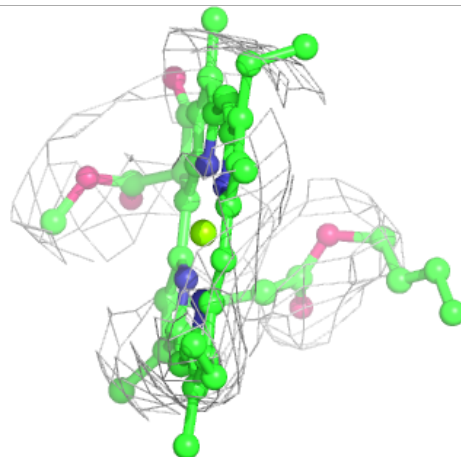
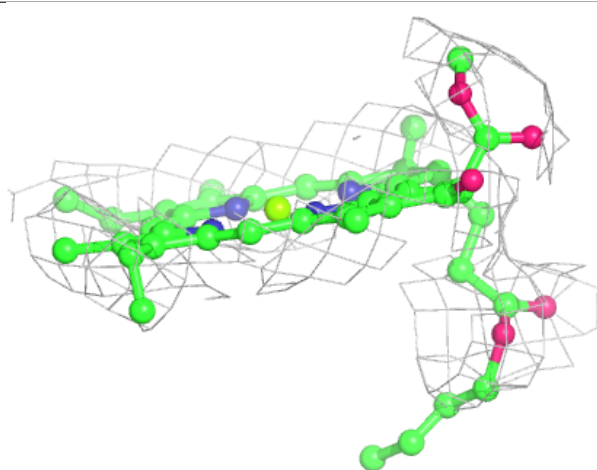
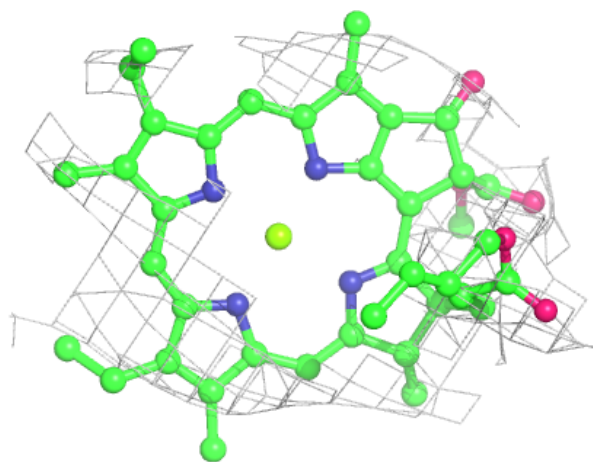
Electron density around CLA B 1235:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



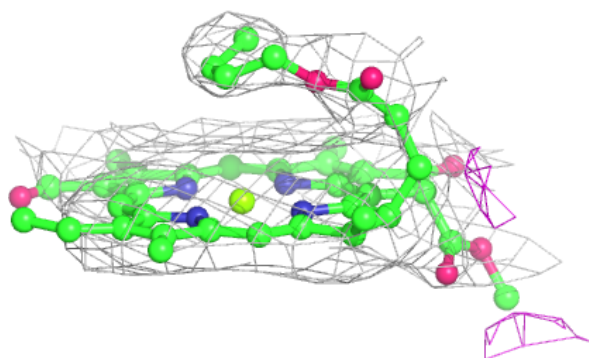
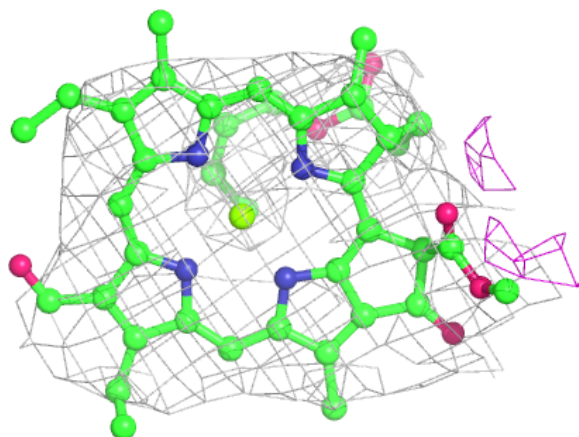
Electron density around CLA B 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

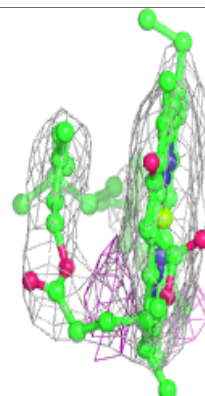
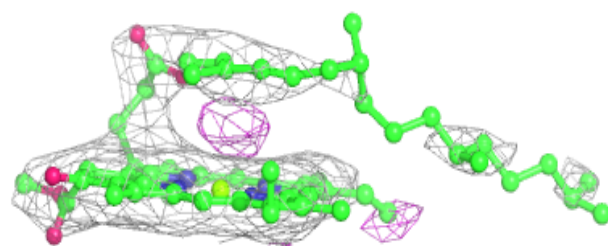
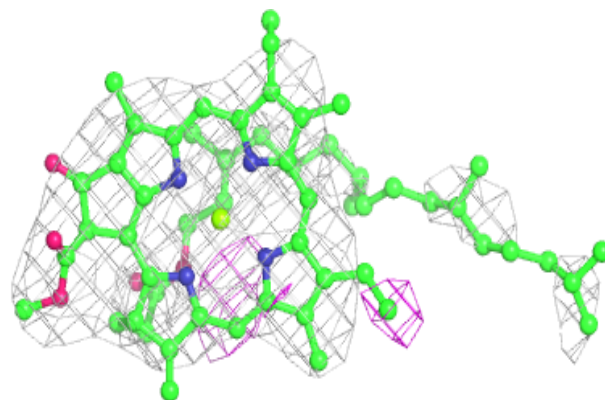


Electron density around CHL 1 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

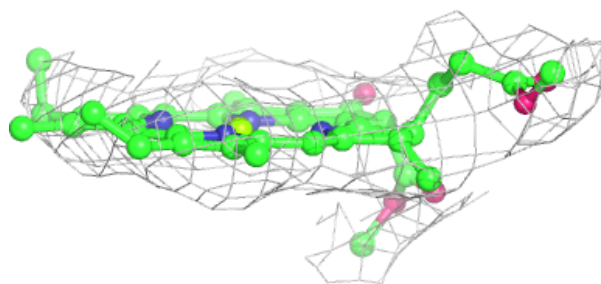
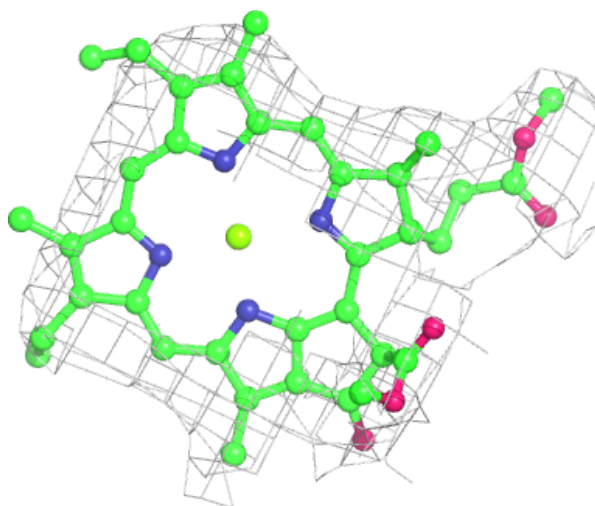
**Electron density around CLA A 1138:**

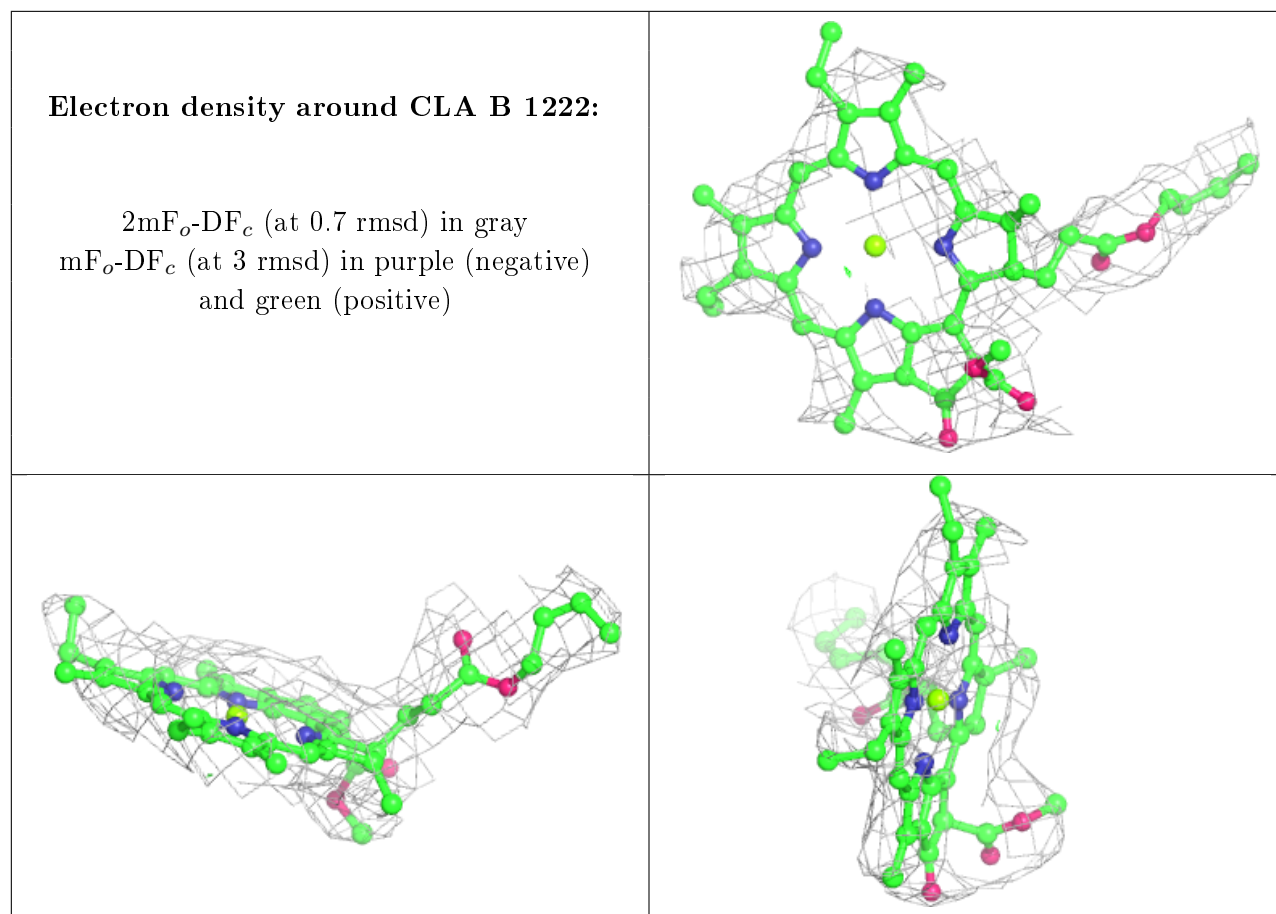
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.